PHYSICAL REVIEW B **78**, 054119 (2008)

Thermal equations of state for titanium obtained by high pressure—temperature diffraction studies

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(Received 27 February 2008; revised manuscript received 20 May 2008; published 22 August 2008)

We have conducted *in situ* high-pressure diffraction experiments on titanium metal at pressures up to 8.2 GPa and temperatures up to 900 K. From the pressure (P)-volume (V)-temperature (T) measurements, thermoelastic parameters were derived for α titanium based on a modified high-T Birch-Murnaghan equation of state and a thermal pressure approach. With the pressure derivative of the bulk modulus, K_0', fixed at 4.0, we obtained: ambient bulk modulus $K_0=114(3)$ GPa, temperature derivative of bulk modulus at constant pressure $(\partial K/\partial T)_P=-1.1(7)\times 10^{-2}$ GPa K^{-1} and at constant volume $(\partial K/\partial T)_V=-9.0\times 10^{-4}$ GPa K^{-1}, volumetric thermal expansivity $\alpha_T=a+bT$ with $a=1.2(\pm 0.6)\times 10^{-5}$ K^{-1} and $b=2.5(\pm 1.1)\times 10^{-8}$ K^{-2}, and the pressure derivative of thermal expansion $(\partial\alpha/\partial P)_T=-8.5\times 10^{-7}$ GPa^{-1} K^{-1}. The ambient bulk modulus and volumetric thermal expansion derived from this work are in good agreement with previous experimental results, whereas all other thermoelastic parameters represent the first determinations for the α phase of titanium. For the ω-phase Ti, we obtained $K_0=107(3)$ GPa and volumetric thermal expansivity at 8.1 GPa $\alpha_T=a+bT$ with $a=6.5(\pm 3.5)\times 10^{-6}$ K^{-1} and $b=2.8(\pm 0.6)\times 10^{-8}$ K^{-2}. Within the experimental uncertainties, the c/a ratios for α-Ti at both room and high temperatures remain constant over the experimental pressures up to 7.8 GPa, presenting a case against the isotropic force potential used in some theoretical modeling for hcp metals under high pressures.

DOI: 10.1103/PhysRevB.78.054119 PACS number(s): 64.30.Ef, 62.50.−p, 61.66.Bi, 62.20.de

I. INTRODUCTION

As a metallic element, titanium is recognized for its high strength-to-weight ratio, the highest among all metals. Chemically, the most noted property of titanium is its excellent resistance to corrosion; it is almost as resistant as platinum, capable of withstanding attack by acids, moist chlorine gas, and by common salt solutions. Because of these unique properties, titanium can be alloyed with other elements such as iron, aluminum, vanadium, and molybdenum, to produce strong lightweight alloys for aerospace, military, industrial processing (e.g., chemicals and petrochemicals), automotive, and other applications.[1]

The fundamental interest in titanium as well as other 3*d* transition metals stems from the fact that they have a narrow *d* band in the midst of a broad *sp* band, which has an impact on their electronic and superconducting properties. The electron transfer from the *s* band to the *d* band under pressure, the so-called *s*-*d* transition, is the driving force behind many structural and electronic transitions in these transition metals[2–7] and also a common feature of many band-structure calculations.[3,4] These studies showed that an increase in the electron number of the *d* band with pressure affects not only the electronic properties but also the stability of the crystal structure. The study of the fundamental thermodynamic properties of titanium, such as equation of state (EOS) and phase transformation, are important not only for a better understanding of its crystal structure, physical chemistry, and mechanical performances and also to the development of theoretical modeling in computational physics.

At ambient conditions, Ti metal crystallizes in a hexagonal close-packed structure (hcp or α phase), and transforms to a body-centered-cubic structure, commonly referred as β phase, at temperatures higher than 1155 K (Ref. 8). With increasing pressure at room temperature, the hcp phase transforms into a hexagonal structure called ω phase, which is not close-packed and has three atoms per unit cell. The pressure induced transition from the α to the ω phase in Ti was first observed by Jamieson[9] and the equilibrium phase boundary is recently determined to be $P(\text{GPa})=5.7+0.0029\times(T-300)$ (K) (Ref. 10). Previous EOS studies have been carried out on the α and ω phases of titanium;[11–14] the pressure-volume measurements, however, were limited to room temperature. In this study, we conducted x-ray diffraction at simultaneously high pressure and high temperature to obtain thermoelastic EOS for the α and ω phases of titanium. The term "thermoelastic" emphasizes the temperature-dependent elastic properties such as temperature derivative of bulk modulus and pressure derivative of thermal expansion. The thermoelasticity is a fundamental property of condensed matter for the modeling of high P-T phenomena under static and dynamic conditions, as well as inside planetary interiors.

II. EXPERIMENT METHODS

The starting titanium metal has an *hcp* structure (α phase) and is in a form of crystalline bulk with a grain size of

~20 microns. The sample is of high purity, with 360 ppm of O, 60 ppm of C, and less than 15 ppm of H, N, Al, V, and Fe as impure ions. Synchrotron x-ray diffraction experiments were conducted using a cubic anvil apparatus[15] at beamline X17B2 of the National Synchrotron Light Source (NSLS), Brookhaven National Laboratory and at beamline BL14B1 of the SPring-8, Japan. An energy-dispersive x-ray method was employed with diffracted x-rays collected at fixed Bragg angles of 2θ=6.4923° at NSLS and 2θ=5.9940° at SPring-8. The cell assemblies used in the experiments are similar to those described in Ref. 15. Briefly, a cubic mixture of amorphous boron and epoxy resin was used as pressure-transmitting medium, and amorphous carbon was used as furnace material. The titanium samples were surrounded by NaCl powders and packed into a cylindrical container of boron nitride (BN), 1.0 mm inner diameter and 2.0 mm length. In each of the two experiments we performed, NaCl was used as an internal pressure standard and temperatures were measured by a W/Re25%-W/Re3% thermocouple. The temperature variations over the entire length of sample container at 1500 K were of the order of 20 K, and the radial temperature gradients were less than 20 K at this condition.[15] X-ray diffraction patterns were obtained for both samples and NaCl in close proximity to the thermocouple junction; errors in temperature measurements were thus estimated to be approximately 10 K.

Pressures were calculated from Decker's equation of state for NaCl (Ref. 16) using lattice parameters determined from x-ray diffraction profiles at each experimental condition. Five NaCl diffraction lines, 111, 200, 220, 222, and 420, were usually used for determination of pressure. The uncertainty in pressure measurements is mainly attributed to statistical variation in the position of diffraction lines and is less than 0.2 GPa in the *P*-*T* range of this study. The effect of deviatoric stress on unit-cell parameters of α-Ti and thermal-expansion data of ω-Ti is minimal because all these data were collected at elevated temperature or on cooling from 900 K, under which the deviatoric stress is expected to be fully relaxed in NaCl and BN (Ref. 17). Under room-temperature compression/decompression without preheating, our cubic cell geometry along with soft materials (NaCl and BN) surrounding the sample would provide a quasihydrostatic pressure environment.[15,17]

In the experiment performed at NSLS, Ti metal was first compressed at room temperature to a desired pressure, followed by stepwise heating to the maximum temperature of 900 K and subsequent cooling to room temperature. The same procedure was repeated several times at progressively higher pressures up to ~8.0 GPa. In the experiment carried out at SPring-8, Ti sample was first compressed at 298 K to the maximum pressure of 7.8 GPa and then heated at a constant loading force. This experiment, cut short due to a thermocouple failure after reaching 973 K, was completed by room-temperature decompression to ambient conditions. Along these experimental *P*-*T* paths, diffraction data were collected for both Ti sample and NaCl under selected conditions.

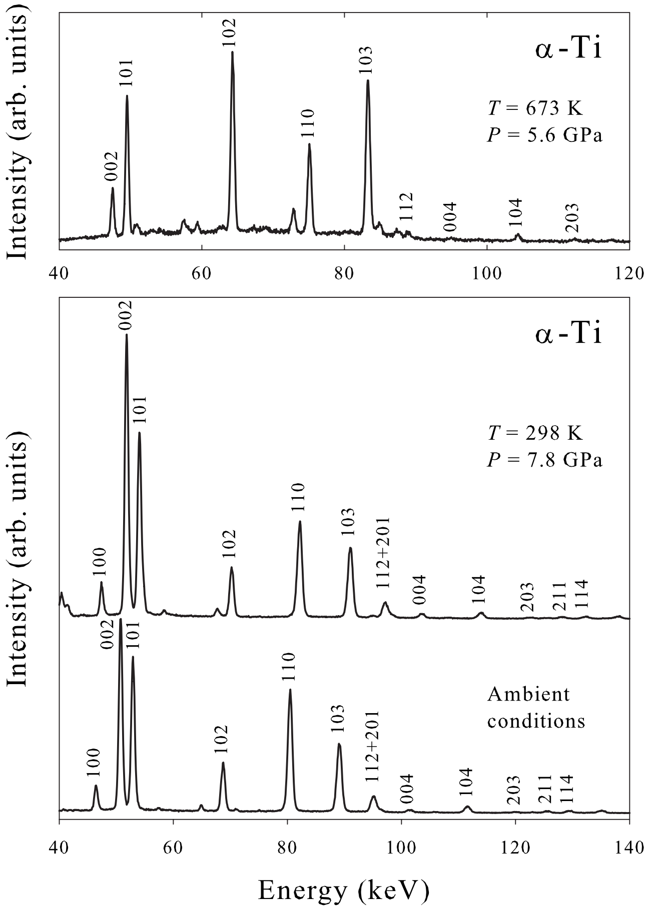

FIG. 1. Representative x-ray diffraction patterns used for the refinement of unit-cell parameters for the α phase of titanium at ambient and high *P*-*T* conditions. The patterns at room temperature (bottom panel) were collected at SPring-8 with the Bragg angle 2θ=5.9940° and the high *P*-*T* pattern was obtained from NSLS with 2θ=6.4923°. The unmarked weak diffraction lines are from boron nitride, which immediately surrounds the titanium sample.

III. THERMAL EQUATION OF STATE OF THE *α*-PHASE TITANIUM

The *in situ* x-ray diffraction experiment on α phase of Ti was performed at pressure and temperature conditions up to 7.2 GPa and 900 K. The x-ray diffraction patterns at selected *P*-*T* conditions are shown in Fig. 1. At ambient conditions, the starting α phase of Ti metal has a unit-cell volume of 35.28(1) Å^3 and lattice parameters α=2.950(1) Å and c =4.680(1) Å, which are in excellent agreement with the JCPDS values (Joint Committee on Powder Diffraction Standards No. 44–1294). The unit-cell volumes are illustrated as a function of pressure and temperature in Fig. 2.

A modified high-temperature Birch-Murnaghan equation of state,[18–20] truncated at third order, was adopted to derive thermoelastic parameters based on the observed pressure-volume-temperature data for the α phase of Ti. A general form of this equation of state is given by

$$P = 3K_T f(1+2f)^{5/2}\left[1 - \tfrac{3}{2}(4-K')f + \ldots\right], \qquad (1)$$

where

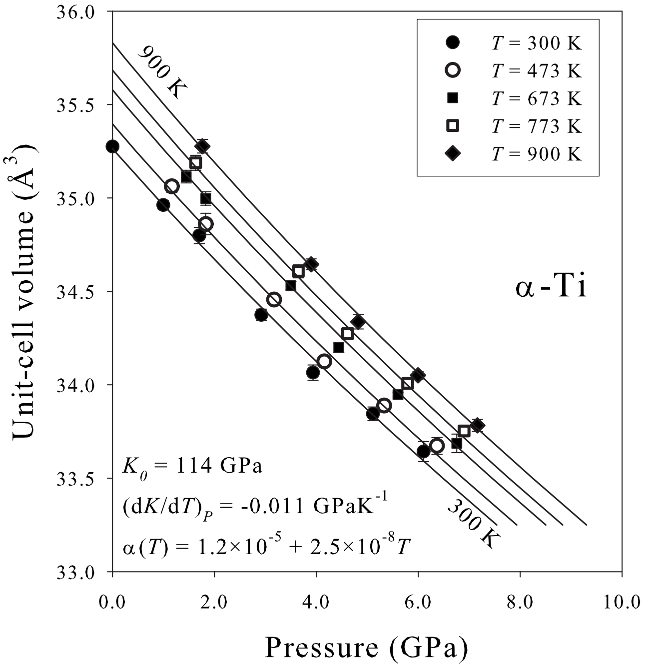

FIG. 2. Pressure-volume-temperature data measured for the α phase of titanium. The curves represent results of the least-squares fit using a modified high-temperature Birch-Murnaghan equation of state at the indicated isotherms.

$$K_T = K_{T_o} + (\partial K/\partial T)(T - 300),$$

$$K' = \partial K/\partial P,$$

$$f = \frac{1}{2}[(V_T/V_{PT})^{2/3} - 1],$$

and

$$V_T = V_o \exp\left(\int \alpha(0,T)dT\right).$$

In Eq. (1), K_{T0} and K_T are isothermal bulk modulus at 300 K and a higher temperature T, and $(\partial K/\partial T)$ and $(\partial K/\partial P)$ are the temperature and pressure derivatives of the bulk modulus, respectively. V_o is the unit-cell volume at ambient conditions, $V_T = V(0,T)$ at atmospheric pressure and a given temperature, $V_{PT} = V(P,T)$ at simultaneously high P-T conditions, and $\alpha(0,T)$ the volumetric thermal expansion at the atmospheric pressure, commonly given in a form of $\alpha(0,T) = a + bT - c/T^2$ (T in Kelvin).[21] Equation (1) modifies the isothermal Birch-Murnaghan equation of state by replacing K_0 with K_T and substituting V_0/V_P with V_T/V_{PT} so that the temperature effects are accounted for. Because of the limited pressure coverage that inhibits an accurate constraint on K' for α-Ti, we assume $K' = 4$ in Eq. (1) throughout the data reduction. Similarly, due to the limited thermal stability of the α-phase titanium, we ignore the c/T^2 term in $\alpha(0,T)$ as well as high-order and cross derivatives of the bulk modulus such as $\partial^2 K/\partial T^2$ and $\partial^2 K/\partial P\,\partial T$.

For the α phase of Ti, all P-V-T data shown in Fig. 2 were collected on cooling (from the peak temperature of 900 K) to minimize deviatoric stress built up during the room-temperature "cold" compression. They were also obtained from a single high P-T experiment at NSLS to eliminate the systematic errors that are typically present among different measurements. As shown in Fig. 2, the collected volume data on α-Ti have good P-T coverage within the stability field of this phase. From a least-squares fit to all P-V-T data (e.g., a "global" fit) using Eq. (1), we obtain $K_o = 114(3)$ GPa, $(\partial K/\partial T)_P = -1.1(\pm 0.7)\times 10^{-2}$ GPa K^{-1}, and $\alpha(0,T) = a + bT$, with $a = 1.2(\pm 0.6)\times 10^{-5}$ K^{-1} and $b = 2.5(\pm 1.1)\times 10^{-8}$ K^{-2}. The errors of thermoelastic parameters throughout this work are those of the least-squares fitting; uncertainties in the measurements of P-V-T were not included for error estimation. As shown in Fig. 2, the thermoelastic parameters derived in the present study produce good fits to the experimental P-V-T data of the α-phase titanium. From the thermodynamic identity:

$$(\partial\alpha/\partial P)_T = (\partial K/\partial T)_P K_{To}^{-2}, \tag{2}$$

the pressure derivative of the volume thermal expansivity, $(\partial\alpha/\partial P)_T$, is found to be -8.5×10^{-7} K^{-1} GPa^{-1}.

The thermal pressure approach to process P-V-T data has been widely applied for its thermodynamic significance.[20,22–25] This approach is also useful for deriving the thermoelastic parameter $(\partial K_T/\partial T)_V$, the temperature derivative of bulk modulus at constant volume, which is experimentally difficult to measure. In this approach, thermal pressure, P_{th}, is calculated as the difference between the measured pressure at a given temperature and the calculated pressure from Eq. (1) at room temperature, with both pressures corresponding to the same volume. Following this definition, thermal pressures are calculated for α-Ti and plotted in Fig. 3. An inspection of Fig. 3 demonstrates that thermal pressures vary linearly with temperature, which is consistent with the linear trends revealed for many different classes of condensed matters (including metals).[22–25] At a given temperature, the thermal pressures show little dependence on volume as they can be approximately fit by a constant value (see insert of Fig. 3).

Thermal pressure at any temperature above 300 K for a given volume can also be analyzed from thermodynamic relations. Following the method of Anderson and his subsequent studies,[22,23] thermal pressure was calculated by

$$\begin{aligned} P_{\mathrm{Th}} &= \int_{300}^{T} (\partial P/\partial T)_V dT = P_{\mathrm{th}}(V,T) - P_{\mathrm{th}}(V,300) \\ &= [\alpha K_T(V_{300},T) + (\partial K_T/\partial T)_V \ln(V_{300}/V)](T-300). \end{aligned} \tag{3}$$

From the least-squares fit of the thermal pressure data of Fig. 3 and the measured volumes (Fig. 2), we obtain average values of $\alpha K_T(V_{300},T)$ and $(\partial K_T/\partial T)_V$ that are 2.82×10^{-3} and -8.98×10^{-4} GPa K^{-1}, respectively, for α titanium. From the thermodynamic identity:

$$(\partial K_T/\partial T)_V = (\partial K_T/\partial T)_P + (\partial K_T/\partial P)_T \alpha K_T(V_{300},T), \tag{4}$$

we obtain a value of -0.012 GPa K^{-1} for $(\partial K_T/\partial T)_P$, which is in excellent agreement with the results derived from Eq.

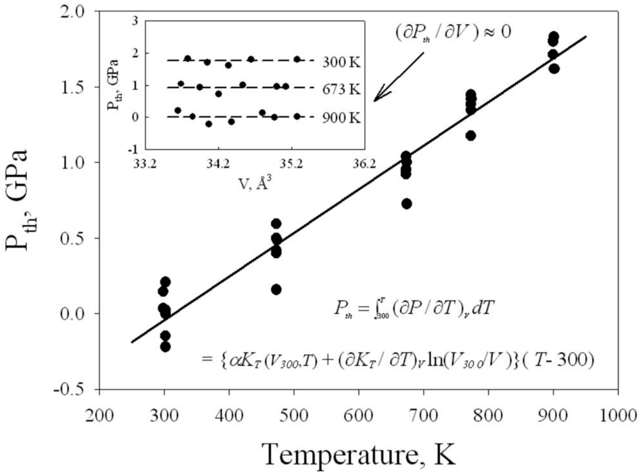

FIG. 3. Thermal pressures (P_{th}) of α titanium as a function of temperature. The spread of the data points at any given temperature corresponds to thermal pressures at different volumes, which is plotted in detail in the insert. The dash lines in the inserted plot show approximate constant values of thermal pressure for a given temperature, indicating that thermal pressure is independent of volume for α titanium. Scattering of data points at room temperature can be taken as uncertainties in thermal pressure calculations from the present *P-V-T* measurements.

(1). The $(\partial\alpha/\partial P)_T$ derived from Eq. (2) is -9.2×10^{-7} K^{-1} GPa^{-1}. An internally consistent thermal equation of state is thus obtained using different methods of analysis for α-Ti.

Several experiments have previously been carried out using diamond anvil cells (DAC) to determine the EOS of α-Ti at room temperature.[11–14] The EOS parameters obtained from these studies are summarized in Table I and are compared with those of the present work. Within the experimental uncertainties, the K_0 value we obtained are in good agreement with those of previous studies (see Table I), whereas the thermoelastic parameters $(\partial K/\partial T)_P$, $(\partial K/\partial T)_V$, and $(\partial\alpha/\partial P)_T$ are determined for the first time for the α phase of titanium.

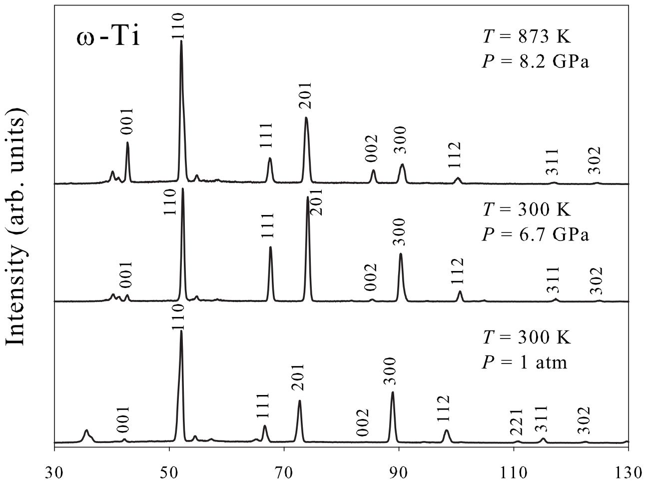

FIG. 4. Representative x-ray diffraction patterns used for the refinement of unit-cell parameters for the ω phase of titanium at selected *P-T* conditions (collected at the Bragg angle $2\theta=5.9940°$). The unmarked weak diffraction lines are from boron nitride, which immediately surrounds the titanium sample.

IV. EQUATION OF STATE AND THERMAL EXPANSION OF THE ω-PHASE TITANIUM

Due to the limited pressure-generating capability of our experimental technique, the *P-V-T* data for the ω-phase Ti could only be obtained at conditions near the ω-β phase-transition phase boundary. For the two experiments performed at NSLS and SPring-8, however, we collected the *P-V* data for the ω-phase titanium on decompression at room temperature. Figure 4 shows the representative x-ray diffraction patterns at selected *P-T* conditions. Consistent with the results of previous studies (e.g., Refs. 9, 11, and 13), the ω phase was retained after pressure is completely released, indicating that the ω phase can be quenched as a metastable phase at ambient conditions. The recovered ω phase of Ti metal has a unit-cell volume of $V=51.86(4)$ Å^3 and lattice parameters $a=4.608(2)$ Å and $c=2.821(2)$ Å from the NSLS experiment, and $V=52.06(6)$ Å^3, $a=4.608(3)$ Å, and $c=2.831(2)$ Å from the SPring-8 experiment.

Figure 5(a) shows the unit-cell volumes of ω-Ti as a function of pressure at room temperature. It is seen that the *P-V* data from the two independent experiments are in good agreement, in both the absolute values and the slopes in the *P-V* plot. The derived EOS parameters from the NSLS and SPring-8 experiments using Eq. (1) are $K_o=108(5)$ GPa and

TABLE I. Summary of the equation of state parameters for α-phase titanium. The values in parentheses are standard deviations and refer to the last digit(s) of the parameters values. The short straight lines indicate the EOS parameters not available from previous studies.

Reference	K_0 GPa	K_0'	$(\partial K/\partial T)_P$ GPa K^{-1}	a, 10^{-5},	b, 10^{-8} $\alpha_T(\mathrm{K}^{-1})=a+bT$	$(\partial\alpha/\partial P)_T$ GPa^{-1} K^{-1}, 10^{-7}	$(\partial K/\partial T)_V$ GPa K^{-1}
This work[a]	114(3)	4.0	−0.011(7)	1.2(6)	2.5(11)	−8.5	–
This work[b]	114(3)	4.0	−0.012(7)	–	–	−9.2	−0.0009
11	119(9)	4.0	–	–	–	–	–
13	102	3.9	–	–	–	–	–
14	109	3.4	–	–	–	–	–

[a] Based on the measured *P-V-T* data of this study and Eqs. (1) and (2).

[b] Thermal pressure approach based on the measured *P-V-T* data of this study and Eqs. (3) and (4).

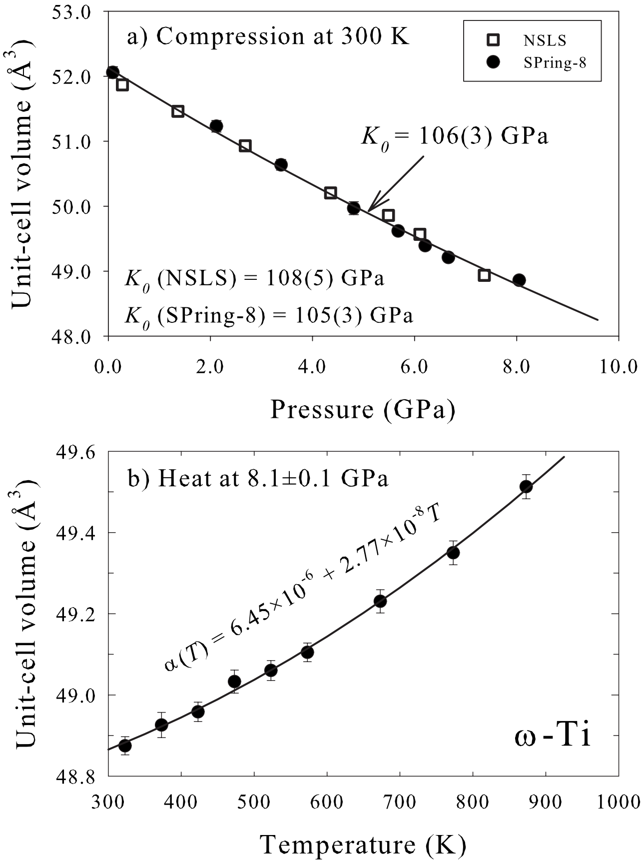

FIG. 5. Unit-cell volumes of ω-phase Ti as functions of pressure at 300 K (upper panel) and temperature at 8.1 GPa (bottom panel).

$K_o=105(3)$ GPa, respectively; and the combined data set yields a value of $K_o=107(3)$ GPa. Within the experimental uncertainties, our results show that the α and ω-Ti have similar bulk modulus (see Table I). The volume data at high P-T conditions are illustrated in Fig. 5(b); upon heating at a constant loading force, the pressures varied only slightly over the temperature range of 300–873 K, approximately 0.1 GPa around a median value of 8.1 GPa, therefore enabling us to derive the isobaric thermal-expansion coefficients at this pressure. From the equation $V_{P,T}=V_{P,0}\exp[\int\alpha_T dT]$, where $V_{P,0}$ and $V_{P,T}$ are, respectively, the unit-cell volumes at 300 K and a given higher temperature under high pressure, we obtained the volumetric thermal expansivity at 8.1 GPa $\alpha_T(\mathrm{K}^{-1})=a+bT$ with $a=6.5(\pm3.5)\times10^{-6}\ \mathrm{K}^{-1}$ and $b=2.8(\pm0.6)\times10^{-8}\ \mathrm{K}^{-2}$. If we assume that α and ω phases of titanium also have similar thermal expansivity at atmospheric pressure, an assumption that warrants further experimental validation, the pressure derivative of thermal expansion for the ω-phase Ti is determined to be $-8.3\times10^{-7}\ \mathrm{K}^{-1}\ \mathrm{GPa}^{-1}$, which is calculated based on the average thermal expansivity over a temperature range of 300–900 K at ambient pressure and 8.1 GPa. From Eq. (2), we obtain $(\partial K_T/\partial T)_P=-0.95\times10^{-2}$ GPa K^{-1}, which is comparable to the derived value for the α-phase Ti.

Previous studies reported bulk modulus of 140 GPa (Ref. 11) and 142 GPa (Ref. 13) for the ω-phase, which are, respectively, 18% and 39% higher than those for the α phase (see Table I). Because all studies reported comparable bulk modulus values for the α-Ti (Table I) and because previous DAC experiments on the ω-Ti were carried out either at pressures where pressure media freeze or on decompression, the bulk modulus discrepancies for the ω-Ti most likely reflect the effect of nonhydrostatic pressures. Under nonhydrostatic conditions, the incident x-ray beam in previous DAC experiments[11–13] was parallel to the maximum stress vector ($\sigma1$) superimposed on the cell geometry, and the lattice planes that satisfied the Bragg law for diffraction are the ones that are perpendicular to the minimum stress vector ($\sigma3$). As a result, the measured lattice volumes and bulk modulus derived from these data would be larger than the hydrostatic values. For the present experiments on ω-Ti, data were collected on decompression without preheating (except for the highest-pressure data points) and hence are also subjected to the effect of nonhydrostatic stress. However, because the incident x-ray beam in our experiments was perpendicular to the maximum stress vector,[26] our experiments would measure the diffraction from the maximum stress direction, which could lead to the bulk modulus that is smaller than the hydrostatic value. The observed discrepancies for ω-Ti can therefore be explained, at least to a qualitative extent, by these differences in diffraction geometry.

V. AXIAL COMPRESSIBILITY OF THE α- AND ω-TITANIUM

At ambient conditions, the α-phase Ti has a c/a ratio of 1.587, far from the ideal value of 1.633 for a hexagonal close-packed crystal structure. This nonideal behavior in hcp metals is generally attributed to the highly anisotropic bonding properties,[27,28] namely, a strongly covalent bond character, with a component aligned along the c axis. The pressure dependence of lattice parameters and the corresponding c/a ratios observed in this study for α-Ti are illustrated in the left panels of Fig. 6. Within the experimental uncertainties, α-Ti exhibits identical axial compressibility along the a and c axis, indicating an isotropic compression of crystal lattice. As a result, the c/a ratios at both room and high temperatures remain constant over the experimental pressures up to 7.8 GPa. By contrast, recent studies in diamond anvil cells[11] revealed that the c/a ratio of the α-Ti increases gradually from 1.583 at atmospheric pressure to 1.622 at 14.5 GPa (see also the bottom left panel of Fig. 6). The gradual increase in the c/a ratio implies an increasingly isotropic interatomic potential, which is important because it validates the isotropic force potential used in some theoretical modeling for elastic modulus of hcp metals under high pressures.[29] Our measurements of α-Ti present a case that does not justify such a treatment. Like for α-Ti, the c/a ratios for ω-Ti also stay constant over the experimental pressures up to 8.1 GPa (the bottom right panel of Fig. 6). For comparison, the c/a ratio in the work of Ref. 11 raises slightly from 0.609 at ambient pressure to a more ideal ratio of 0.613 at 16 GPa.

Radial diffraction geometry in DAC is an emerging and advanced technique that allows measurements in the maximum, minimum, and hydrostatic stress directions. A recent study using this technique on osmium, also an hcp metal, revealed a constant c/a ratio up to 30 GPa along hydrostatic

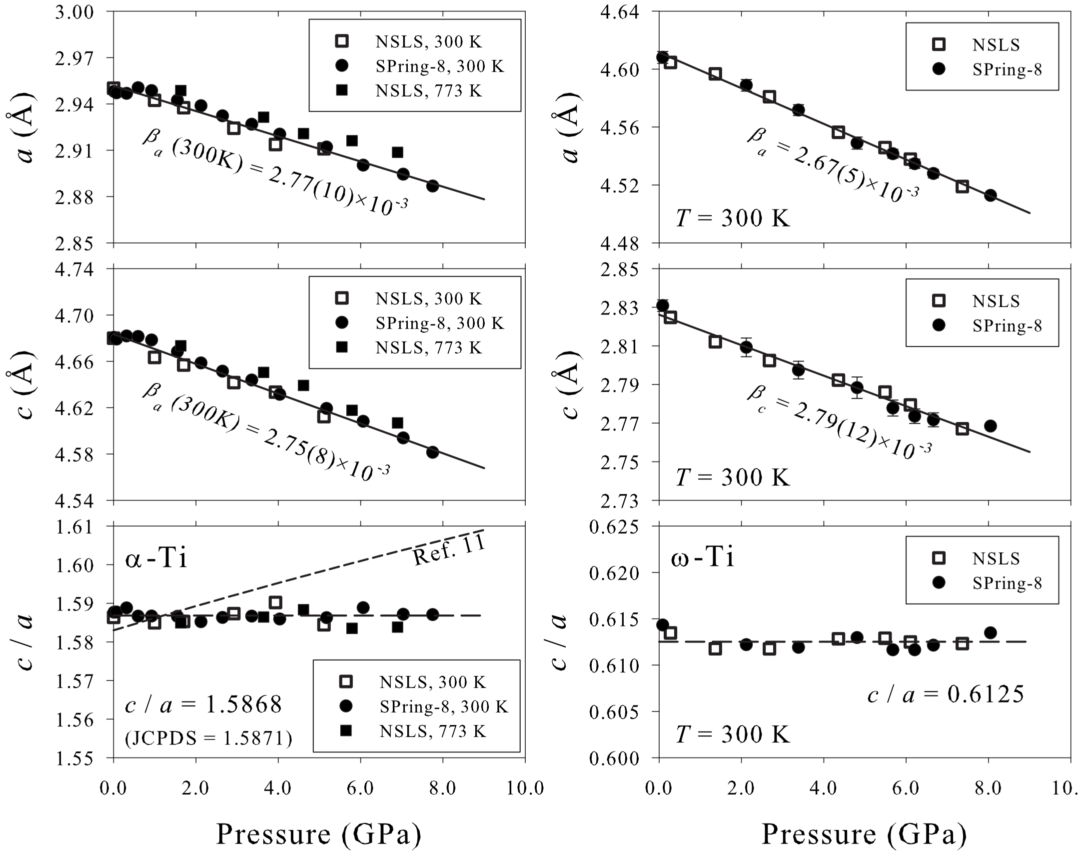

FIG. 6. Variation of lattice parameters as a function of pressure for α-Ti (left panels) and ω-Ti (right panels) at selected temperature conditions from the NSLS (squares) and SPring-8 (circles) experiments. These observations reveal the identical axial compressibility along the a and c axis for both α and ω-Ti and hence constant c/a ratios over the experimental pressures up to 8.1 GPa. JCPDS refers to Joint Committee on Powder Diffraction Standards (No. 44–1294).

stress direction.[30] More importantly, this work showed that up to 15 GPa the c/a ratios in the minimum and maximum stress directions agreed well with the hydrostatic values; at higher pressures, however, the apparent c/a ratios increased in the minimum stress direction and decreased in the maximum stress direction. In addition, the observed increase in the apparent c/a ratios in the minimum stress direction is consistent with the variation of c/a ratios measured in conventional diamond cell experiments where the incident x-rays are parallel to the loading direction.[31] This suggests that, above the pressure where all known pressure media freeze (~15 GPa), the experiments are actually nonhydrostatic. As a result, data collected from the experiments that are intended to be hydrostatic have in fact measured diffraction from the minimum stress direction, therefore resulting in increased apparent c/a ratios. Based on these observations, an increase in the c/a ratio would be expected if previous DAC experiments on Ti were under nonhydrostatic conditions, either because of the freezing or leaking of pressure media. The constant c/a ratios were observed in the present study because our pressure-loading system provides the uniform compression in all six directions of a cubic cell, in contrast to the uniaxial compression in nonhydrostatic DAC experiments. In addition, heating is an effective approach to relax the deviatoric stress built up during room-temperature compression/decompression. Clearly, nonhydrostatic pressure contributions need to be carefully studied to correctly interpret and compare the lattice-parameters determinations and, in the present case, the c/a ratios measured using different high-pressure diffraction techniques.

VI. CONCLUSION

In summary, we have conducted *in situ* x-ray diffraction experiments on titanium metal at pressures up to 8.2 GPa and temperatures up to 900 K. From these measurements, we have derived thermal equations of state for the α and ω titanium, which includes temperature and pressure derivatives of thermal expansion and elastic bulk modulus. Our data also present a case against the isotropic force potential used in some theoretical modeling for hcp metals under high pressures. These results extend our knowledge of the fundamental thermophysical properties on titanium metal and are important to the understanding of the phase stability of different titanium phases and to improve the theoretical modeling of these materials under dynamic conditions.

ACKNOWLEDGMENTS

This research was supported by the Los Alamos National Laboratory, which is operated by Los Alamos National Security LLC under DOE Contract No. DE-AC52-06NA25396.

The experimental work was carried out at the beamline X17B2 of National Synchrotron Light Source of Brookhaven National Laboratory, which was supported by the Consortium for Materials Properties Research in Earth Sciences (COMPRES) under NSF Cooperative Agreement EAR 01-35554, and at the beamline BL14B1 of SPring-8, which was supported by Synchrotron Radiation Research Center, Japan Atomic Energy Research Institute.

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