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Disclaimer

A study of tantalum pentoxide Ta_2O_5 structures up to 28 GPa

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Tantalum pentoxide Ta_2O_5 with the orthorhombic L-Ta_2O_5 structure has been experimentally studied up to 28.3 GPa (at ambient temperature) using synchrotron angle-dispersive powder x-ray diffraction (XRD). The ambient pressure phase remains stable up to 25 GPa where with increased pressure a crystalline to amorphous phase transition occurs. A detailed equation of state (EOS), including pressure dependent lattice parameters are reported. The results of this study were compared with a previous high-pressure XRD study by Li *et al.* A clear discrepancy between the ambient-pressure crystal structures and, consequently, the reported EOSs between the two studies was revealed. The origin of this discrepancy is attributed to the different crystal structures used to index the XRD patterns.

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I. INTRODUCTION

Tantalum pentoxide Ta_2O_5 has been extensively studied mainly due to its high refractive index, making it suitable for optical coating,[1,2] and its wide bandgap (Eg = 4 eV) and dielectric constants, making it suitable in electronic applications such as capacitors.[3] Previous studies on the effect of the residual stress in the case of Ta_2O_5 films suggested a strong pressure dependence of the bandgap and residual stress was shown to be the main reason for a crystalline to amorphous transition at about 18GPa.[4] In this context, quasi-hydrostatic pressure is widely used to mimic strain and residual stress in films of various systems. Moreover, the properties of Ta_2O_5 are important for a number of practical applications, including some, *e.g.* energetic materials, that require knowledge of its high pressure equation of state (EOS). Classical energetic materials are organic molecular compounds such as 2,4,6-trinitrotoluene (TNT), Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX), etc., which have a wide range of industrial and defense uses due to their stored and easily available chemical energy. An attractive way of increasing the energy density of these materials is through the addition of metallic powders, which can provide significantly more energy through oxidation. Aluminum (Al), silicon (Si), boron (B) have been widely studied in this context, and with the advent of nanopowder production technologies, many other metals are currently being considered.[5,6] In the nanometer domain even nominally refractory metals such as tantalum (Ta) may be amenable to explosives and propellants applications.[6] Ta and its oxidation have already been studied for example in thermite reactions.[7] Understanding and modeling the behavior and effects of metal fuels under these usage scenarios requires information on the properties of their oxides, including in particular the EOS. Experimental measurements of the structure and equation of state of Ta_2O_5 at moderate pressures are however rather scarce, despite ongoing interest in its shock properties under low initial density conditions, e.g. powders and aerogels.[8,9]

The crystal structure of tantalum pentoxide at ambient conditions has been under long debate, mainly due to the difficulty to grow high quality single crystals. Nevertheless, two, so-called "low-temperature", ambient condition crystal structures are widely accepted in the literature:[10,11] a) the orthorhombic *P2mm* (S.G. 25, Z=11, PDF-71-639,ICSD 9112) L-Ta_2O_5[12] and b) the orthorhombic *Pccm* (S.G. 49, Z=2, PDF-01-070-9177, ICSD 95462) β-Ta_2O_5.[13] Moreover, a plethora of high-temperature structures have been reported. Here,

for simplicity, we will only refer to the orthorhombic *Pmm2* (S.G. 25, Z=12, PDF-79-1375, ICSD 66366) T-Ta_2O_5 structure synthesized by Hummel *et al.*[14] through high temperature chemical procedures using an intermediate TT-Ta_2O_5 phase as a percussor. L-Ta_2O_5 and T-Ta_2O_5 share common structural characteristics, which are the presence of edge and corner sharing TaO_6 octahedra and TaO_7 pentagonal bipyramids.[12,14,15] Ta and O atoms form O-Ta-O layers in the *ab* plane and along the *c* axis. The TaO_6 octahedra and TaO_7 pentagonal bipyramids of adjacent layers are connected by corner sharing along the c axis, see Fig. 1. In contrast, only corner sharing TaO_6 octahedra are present in the β-Ta_2O_5 structure,[13] see Fig. 1(b).

To our knowledge, only one high pressure study on bulk Ta_2O_5 has been published, by Li *et al.*[15] using in situ synchrotron X-ray diffraction (XRD) and Raman spectroscopy. In the same study the EOS of Ta_2O_5 up to 12 GPa, including pressure dependent lattice parameters, was reported. Moreover, a pressure induced structural transition of the starting orthorhombic phase to an amorphous form in the pressure range of 18.4 - 24.7 GPa has been observed. In their study, although the authors state that they present a high pressure study of the low-temperature orthorhombic Ta_2O_5, the reported cell volume and lattice parameters are in strong disagreement with those reported by Stephenson *et al.*[12] and Aleshina *et al.*.[13] Instead, it seems that Li *et al.*[15] used the T-Ta_2O_5 structure to index their high-pressure XRD patterns. We believe this in an important shortcoming that should be corrected, not only for the accurate knowledge of the EOS of Ta_2O_5, but also because future studies in other systems may be based on the results reported by Li et al. In order to resolve this issue, we have carried out a detailed synchrotron angle-dispersive powder XRD study of Ta_2O_5 up to 28.3 GPa. We show that the XRD patterns of commercially available Ta_2O_5 can be well indexed with the low temperature orthorhombic L-Ta_2O_5 in agrement with Stephenson *et al.*.[12] Moreover, we report a detailed EOS of the L-Ta_2O_5 up to 25 GPa and a pressure induced amorphization above this pressure.

II. METHODS

High purity and commercially available (>99.99% CERAC, INC.) Ta_2O_5 was ground to a fine powder for x-ray diffraction (XRD) measurements. The sample including pressure sensors were loaded into diamond-anvil cell (DAC) sample chambers. Rhenium gaskets

(preindented to 40-45 μm thick using 400 μm diameter culets) were used to radially confine the pressurized samples. Initial sample chamber diameters were nominally 150 μm. Ne was utilized as a pressure-transmitting medium (PTM) for XRD. Pressure was determined using a known ambient temperature EOS of gold[16] and also using a calibrated ruby luminescence scale.[17] An image plate CCD detector was used to collect pressure dependent X-ray diffraction data at the Advanced Light Source Beamline 12.2.2. An X-ray wavelength of $\lambda = 0.4959$Å was selected using a Si(111) double-crystal monochromator. Exposures time varied between 10 and 30 secs. The sample to detector distance of 300 mm was determined using a CeO_2 (or LaB_6) diffraction pattern. The X-ray beam was focused to 10 x 10 μm using Kirkpatrick-Baez mirrors. More details on the experimental set up are given in Kunz *et al.*.[18]

Integration of powder diffraction images to yield scattering intensity versus 2θ patterns and initial analysis were performed using the DIOPTAS[19] program. Calculated XRD patterns were produced using the POWDER CELL program,[20] for the corresponding crystal structures according to the EOSs determined experimentally in this study and also for the previously published crystalline structures all assuming continuous Debye rings of uniform intensity. Le Bail refinements were performed using the GSAS[21] software. Indexing of XRD patterns has been performed using the DICVOL program[22] as implemented in the FullProf Suite.

III. RESULTS AND DISCUSSION

In Fig. 2(a), we plot the comparison between the experimental XRD pattern of Ta_2O_5 with the calculated pattern of L-Ta_2O_5 at ambient pressure. An almost perfect match, apart from a slight difference in relative intensities, is clearly observed. This is better highlighted by the Rietveld refinement given in Fig. 2(b). The cell volume and the lattice parameters obtained for Ta_2O_5 in this study are in excellent agrement with those reported by Stephenson *et al.* for L-Ta_2O_5, see Table I. We present in Fig. 3 the integrated diffraction patterns of Ta_2O_5 at selected pressures up to 28.3 GPa. The L-Ta_2O_5 phase appears to remain stable up to 26.5 GPa followed by a pressure induced amorphization at higher pressures, see Fig. 3. With complete pressure release the amorphization is only partially lifted.

From the XRD data of Ta_2O_5, we determined the pressure dependent lattice parameters

TABLE I. Experimental structural parameters of L-Ta_2O_5 and T-Ta_2O_5 phases of Ta_2O_5 at ambient pressure. Listed parameters include space group (SG), number of formula units in the unit cell Z, lattice parameters, cell volume, and the zero pressure bulk modulus, K_o, derived from unweighted fits to the third-order Birch-Murnaghan EOS model.

Reference	Crystal structure	SG	Z	a(Å)	b(Å)	c(Å)	V_o(Å^3)	K_o
Stephenson et al.	L-Ta_2O_5	*P2mm*	11	6.198(5)	40.290(33)	3.888(5)	970.9	-
Hummel *et al.*	T-Ta_2O_5	*Pmm2*	12	43.996	3.894	6.209	1063.75	-
Li *et al.*	T-Ta_2O_5	*Pmm2*	12	43.997	3.894	6.209	1063.75	139
This Study	L-Ta_2O_5	*P2mm*	11	6.197(6)	40.32(2)	3.813(4)	972.9(18)	199

and cell volumes, see Fig. 4. We were not able to determine the positional parameters for all atoms (*i.e.* only the positional parameters of Ta cations were refined during the Rietveld refinement), and consequently the interatomic distances, due to: a) the large difference in the Z values between Ta and O and b) the significant number (>100) of free positional parameters. The results are compared with those published by Stephenson *et al.* shown in Figures 4. Close inspection of the compressibility of the normalized lattice parameters (Fig. 4(a)) reveals a much higher compressibility along the c-axis, reflecting the higher compressibility perpendicular to the layers, see Fig. 1(a)). Moreover, the axes compressibility is marketly reduced in the pressure range between ∼16GPa (a-axis) and ∼22GPa (b and c-axes). Consistent with most high-pressure EOS studies, we conducted unweighted fits (Vo is a fixed parameter) of the pressure-volume data, to a third- and second-order Birch-Murnaghan (B-M) equations of state[23] and determined the bulk modulus K_o and its first derivative K' (for the third-order B-M) at zero pressure for the L-Ta_2O_5. Although the XRD patterns of Ta_2O_5 appear to be that of a pure crystalline phase up to 25.5 GPa, we cannot completely exclude that the gradual pressure induced amorphization starts at lower pressures. For this reason, and in order to rule out any possible effect on the reported EOS, we only included pressure-volume data up to 22 GPa in our analysis. The elastic parameters obtained this way are: a) K_o= 199±2GPa and K'=0.1 for the third-order B-M and b) K_o= 160±5GPa for the second-order B-M. We postpone the discussion about the very low value of the K' as determined by the third-order B-M; however, we would like to note that the

results of the third-order B-M fit should be only considered as indicative of a low K', given that its applicability range is limited to $K' \geq 4$.

To gain deeper insight into how Ta_2O_5 responds under quasi-static compression, we conducted weighted fits and used the reduced χ^2_{red} goodness-of-fit formalism to compare the effectiveness of three EOS models to represent the P-V data. The reduced χ^2 value closest to 1 represents the best-fit model, see Ref.[24] for a complete description of the procedure. The Birch-Murnaghan,[23] (B-M), 2^{nd} to 4^{th} orders, the Vinet,[25] and the F-f[26] finite strain 1^{st} order EOS models were fit to the data, see Fig. 5. Corresponding two-dimensional confidence ellipses are plotted for the best fit model to reveal two-variable correlation information (See Figs. 6(a) and 6(b)). Bivariable confidence plots enable a more comprehensive basis for comparison of EOS parameters to alternative theoretical and/or experimental results.[27] Application of the F-f model to the data reveals that the pressure dependent stress, within the established errors, exhibits a linear response to applied strain (See Fig. 5(b)). There is no indication of a pressure or strain induced modification of the initial structure. The third-order B-M EOS and the first-order F-f EOS models yielded the statistically best representations of the data (See: Figure 5(a) and Table II). It is unusual that the first pressure derivative of the bulk modulus, K', has a value near zero; within the experimental error, the pressure dependent compressibility of Ta_2O_5 appears to be pressure invariant or unchanged up to approximately 25 GPa.

TABLE II. Model EOS parameters derived from fits to our Ta_2O_5 data, weighted according to experimental uncertainties. Note: *K"* (bracketed terms) is implied for 2nd and 3rd B-M and F(f) 1^{st} order results (See: O.L. Anderson, 1995 Oxford Univ. Press[28]). According to the method outlined by R.J. Angel, and with exception to the F-f EOS model, Vo is a floating parameter in EOS model fitting.[27]

Experimentally Weighted Fits											
B-M order	V_0(Å^3)	V_0 esd	K_0(GPa)	K_0 esd	K'	K' esd	K"	K" esd	χ^2_{red}	Max ΔP (GPa)	KS-test
2	973.94	0.73	172.57	5.93	4.00	0.00	[-0.02]	[0.00]	4.48	3.48	0.40
3	973.57	0.55	209.07	7.91	-0.88	0.60	[-0.11]	[0.03]	1.50	2.71	0.18
4	973.22	0.45	249.05	13.78	-8.60	2.10	0.02	0.05	0.54	1.01	0.18
Vinet EOS	V_0	V_0 esd	K_0	K_0 esd	K'	K' esd	K"	K" esd	χ^2_{red}	Max ΔP	KS-test
	973.44	0.51	214.49	9.03	- 2.97	0.94	[0.00]	[0.00]	1.30	2.71	0.16
F-f order	V_0	V_0 esd	K_0	K_0 esd	K'	K' esd	K"	K" esd	χ^2_{red}	Max ΔP	KS-test
1	972.87	[1.00]	202.22	4.36	-0.25	0.35	[-0.09]	[0.01]	0.61	0.92	0.34

The low value of K' as determined by both the unweighed and the weighed fits is relatively unusual; however, low or even negative values of K' have been reported in the literature.[29,30] The complete elucidation of this aspect is beyond the scope of this paper as it may require singe crystal diffraction in order to accurately determine interatomic distances and also thermal expansion measurements. At the present level, we can speculate on the following two explanations. One is that the L-Ta_2O_5 crystal structure is characterized by extensive corner-sharings between TaO_x polyhedra with additional open space between the polyhedra. Consequently, the compressibility is governed primarily by changes in Ta-O-Ta bond angles through rotation of multiple corner sharing polyhedra. This is in agrement with the experimentally observed higher compressibility of the c axis, see Figs. 1 and 4, the axis that is perpendicular to the O-Ta-O layers. Another way to describe the same scenario is the, almost negligible, repulsion between polyhedra as discussed in details in Ref..[24] A second explanation is the onset of pressure induced Bragg peak broadening, which even during the initial step of compression, signals that L-Ta_2O_5 exhibits a tendency for disorder even at low pressures. The proposed tendency for disorder is in agrement with the results of the Raman spectroscopy measurements by Li *et al.*[15] This is probably, due to pressure induced frustration and/or competition between different local orderings of the Ta sublattice, as XRD intensity is, almost entirely, dominated by Ta cations. Finally, we cannot completely exclude the possibility that the extremely low K' is partially an artifact due to the pressure induced peak broadening which affects the accuracy of the p-V data.

Now we turn our attention to the disagreement between the EOS reported in our study and the one reported by Li *et al.* . Although the authors in Ref.[15] state that they present a high pressure study of the low temperature orthorhombic Ta_2O_5 they used the T-Ta_2O_5 structure for indexing their XRD patterns and further reported volumes and lattice parameters that are in agrement with the those reported by Hummel *et al.*, see Table I. Given that the authors used commercially available Ta_2O_5 powder, it is unlikely that the starting material is the T-Ta_2O_5 allotrope, which is normally synthesized under specific chemical and temperature conditions. As clearly observed in Fig. 2(a), the calculated XRD patterns of L-Ta_2O_5 and T-Ta_2O_5 are hardy distinguishable based only on the positions and the relative intensities of the main Bragg peaks. This can be attributed to the common structural characteristics of these two allotropes,[12,14] see discussion in the introduction and Table I. However, a closer inspection of the lower intensity Bragg peaks, especially at low 2θ, can

provide a way to distinguish between the XRD patterns of these structural modifications, see inset in Fig.2(a). Unfortunately, a refinement of the experimental patterns was not provided by the authors and moreover, the low angle region of the 2θ range ($<8^o$ in Ref. 1 and $< 6.4^o$ in Fig. 2(a)) is missing. Nevertheless, we believe that the measured XRD pattern by Li *et al.* can be more optimally indexed with the L-Ta_2O_5 structure. From the above discussion, we conclude that Li and coworkers made an unintentional error by indexing their experimental patterns with the T-Ta_2O_5 structure and thus, reported an EOS that doesn't correspond to any crystal form of Ta_2O_5. Finally, it is plausible to assume that the higher critical pressure for amorphization in this study (26.5 GPa vs ∼21 GPa in Ref.[15]) can be attributed to the use of neon as a PTM in this study compared to the significantly less hydrostatic (above 10 GPa) methanol-ethanol mixture[31,32] used by Li *et al.*

IV. CONCLUSION

To summarize, the high-pressure structural of Ta_2O_5 has been explored experimentally up to 28.3 GPa using synchrotron x-ray diffraction. We have shown that the ambient phase can be more appropriately indexed with the "low-temperature" L-Ta_2O_5 structure. The L-Ta_2O_5 phase remains stable up to 25 GPa were pressure induced amorphization takes place. The respective bulk moduli and corresponding pressure derivatives were derived from weighted and unweighted fits using selected (relatively optimal) EOS models. We have shown that Li and co-workers have unintentionally reported an erroneous high-pressure EOS for the low temperature phase of Ta_2O_5 based on the T-Ta_2O_5 phase.

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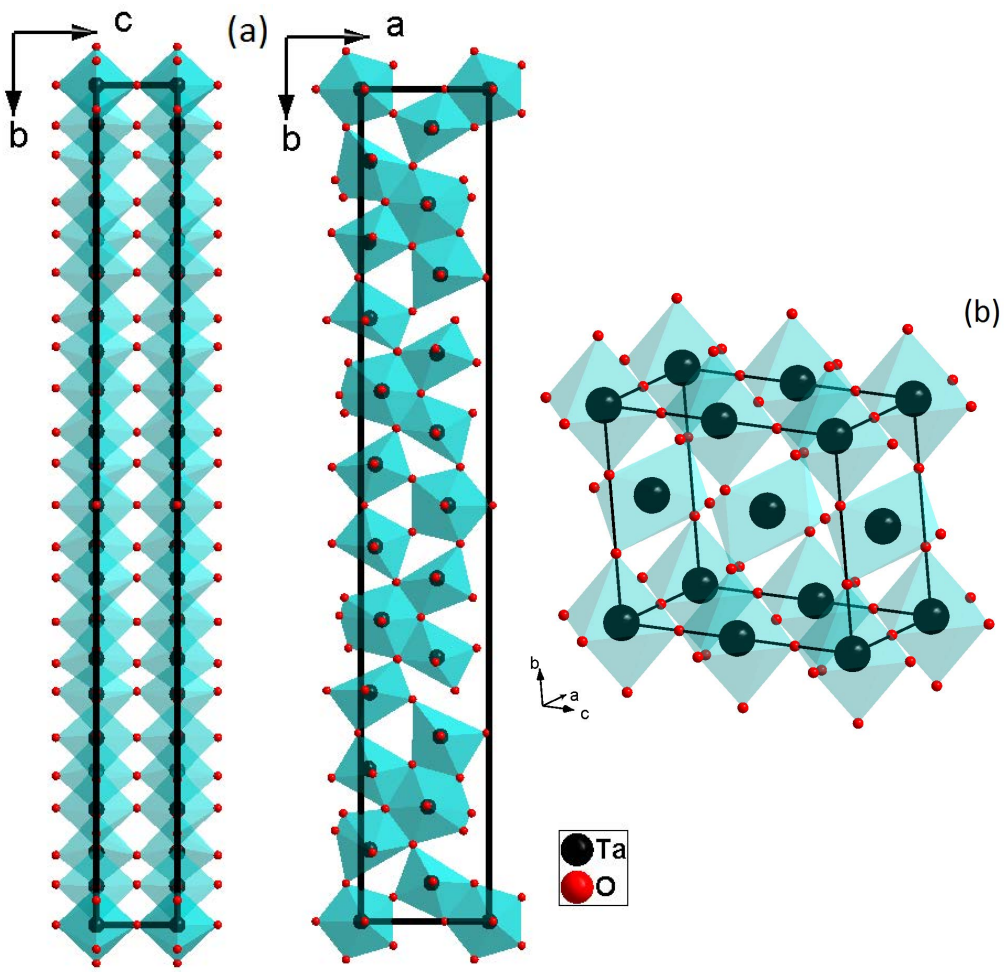

FIG. 1. Schematic representations of: a) the L-Ta_2O_5 structure along the a (left) and c (right) axis and b) the β-Ta_2O_5.

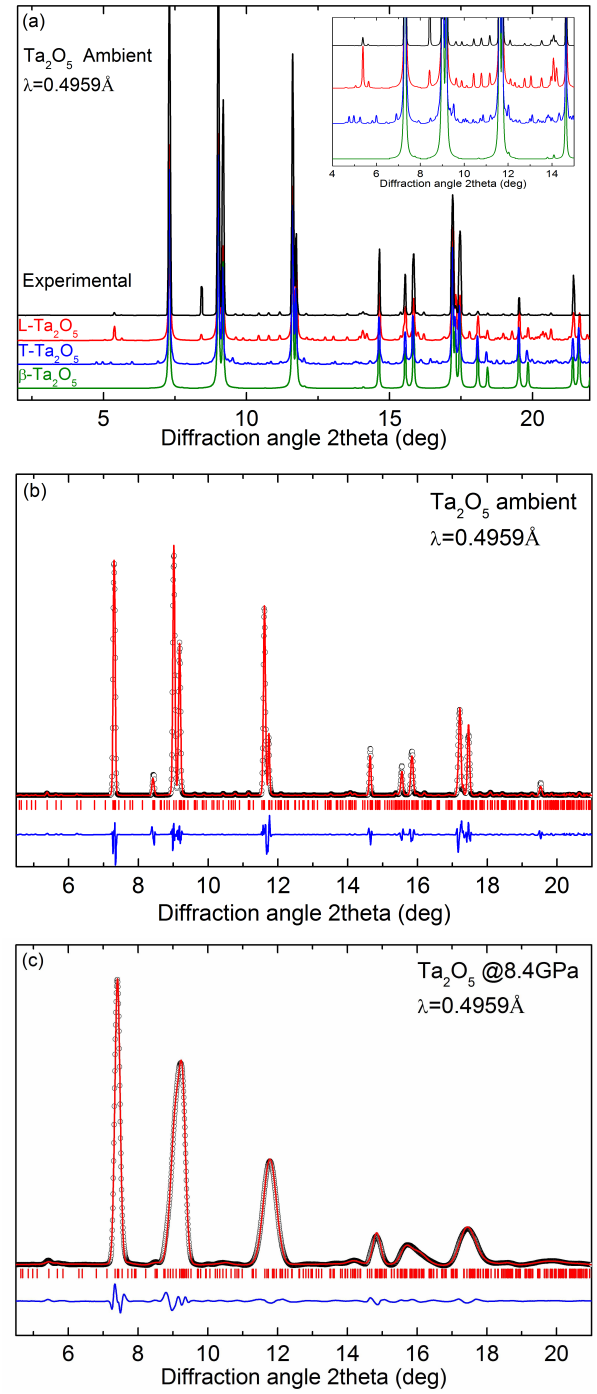

FIG. 2. (a) Calculated XRD patterns of L-Ta_2O_5, β-Ta_2O_5 and T-Ta_2O_5 at ambient pressure. The experimental XRD pattern of this study is also shown. (b) Rietveld refinement results for Ta_2O_5 at ambient pressure and (c) at 8.4 GPa, L-Ta_2O_5 structure. Symbols correspond to the measured profile, the red solid lines represent the results of Rietveld refinements. The difference curve (blue curve) is also plotted. Vertical tick marks indicate Bragg peak positions.

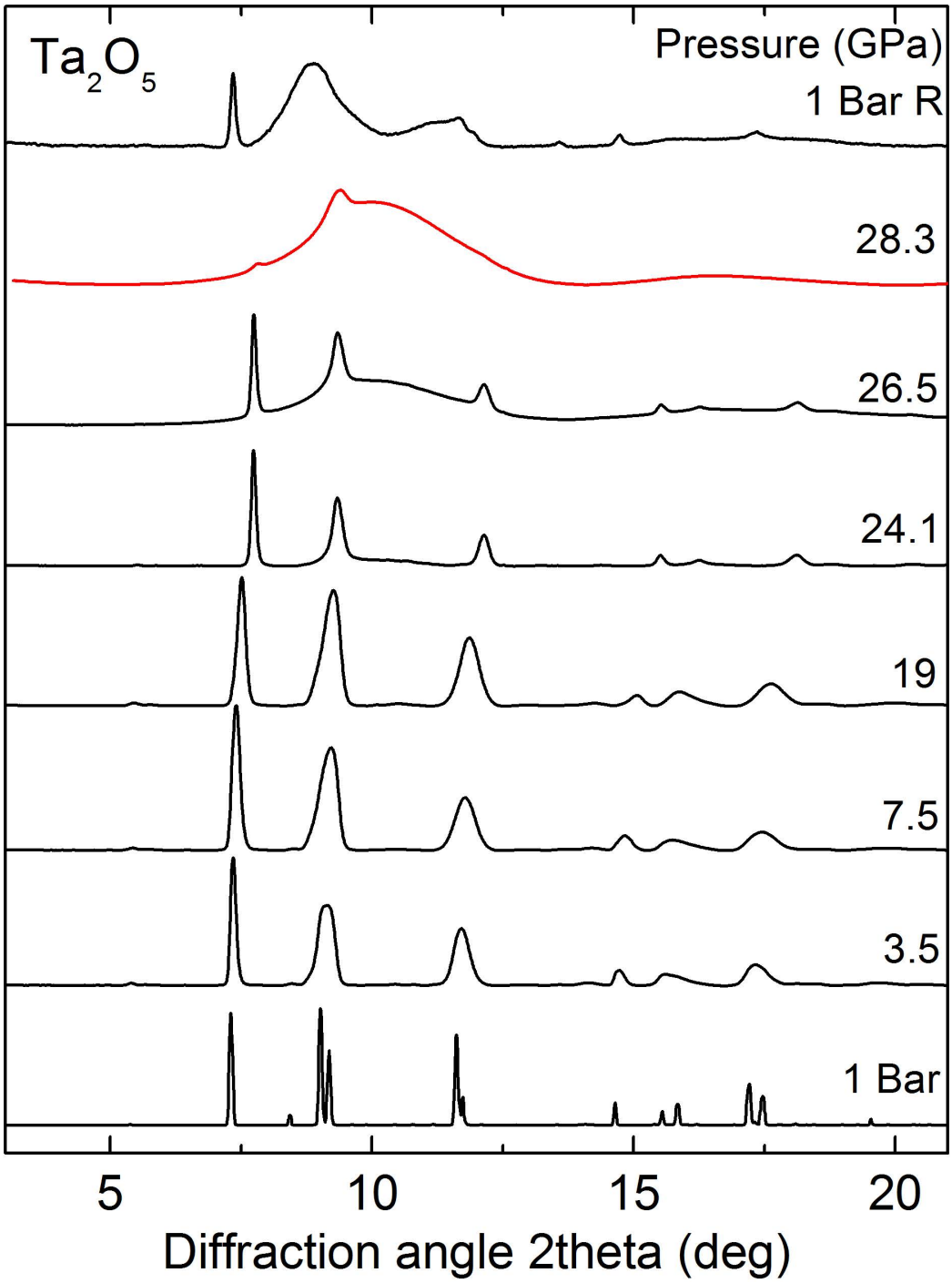

FIG. 3. XRD patterns of Ta_2O_5 at selected pressures.

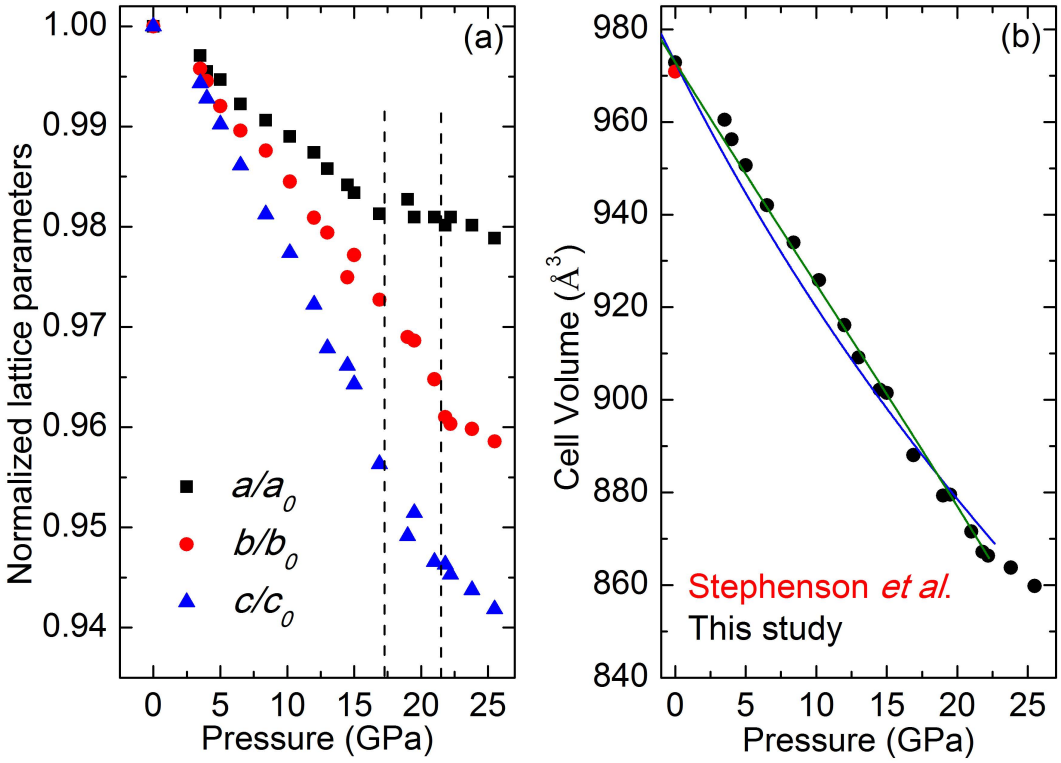

FIG. 4. (a) Pressure dependence of the normalized lattice parameters and (b) pressure-volume data for the L-Ta_2O_5. The solid green and blue lines are third- and second-order B-M equation of state unweighted fits respectively, of the L-Ta_2O_5 phase experimental data; Vo was a fixed fitting parameter. The vertical dashed lines in (a) mark the pressure range of the observed decrease of the axes compressibility, see text for details.

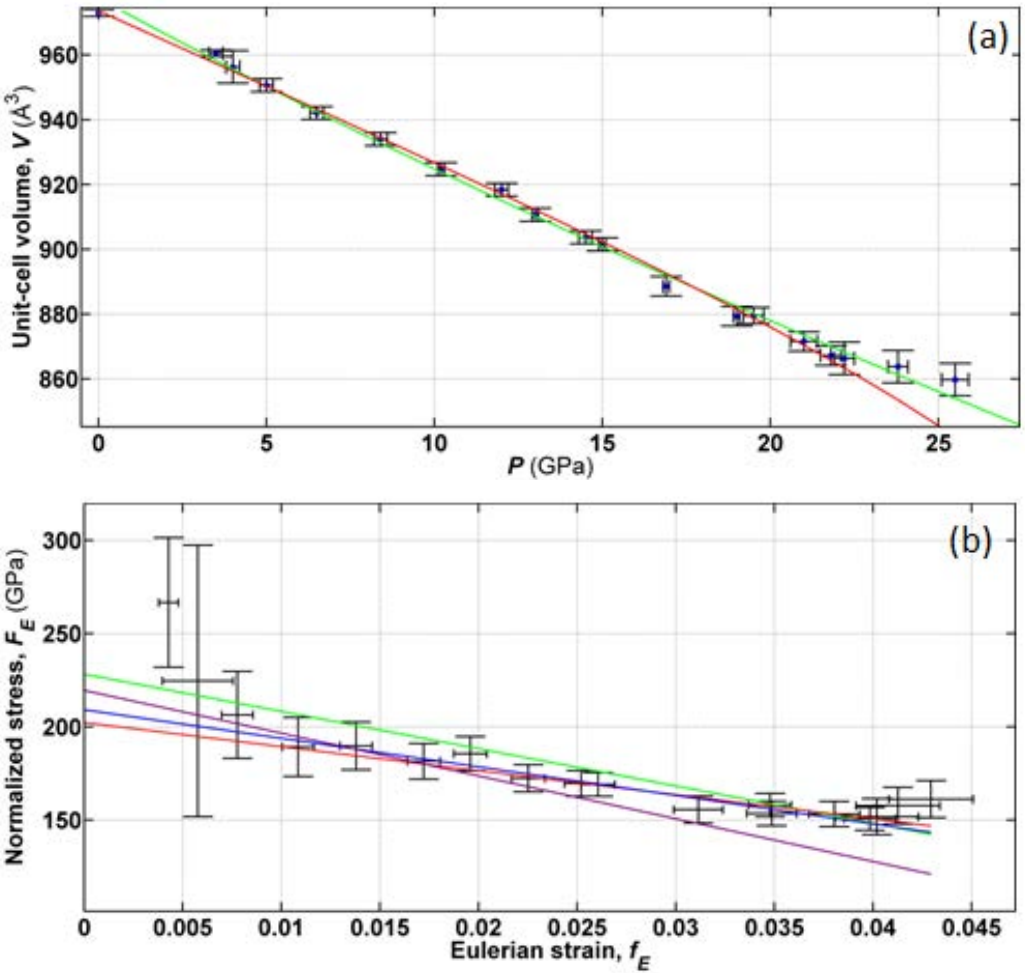

FIG. 5. (a) Third order Birch-Murnaghan EOS model weighted fit to Ta_2O_5 data. The red line represents a weighted fit and the green line is from an unweighted fit. b) First-order F-f EOS model weighted fit to Ta_2O_5 data. The red line represents a weighted fit and the green line is from an unweighted fit. The violet line represents a weighted Vinet EOS fit and the blue line is from a third-order B-M EOS model fit to the data.

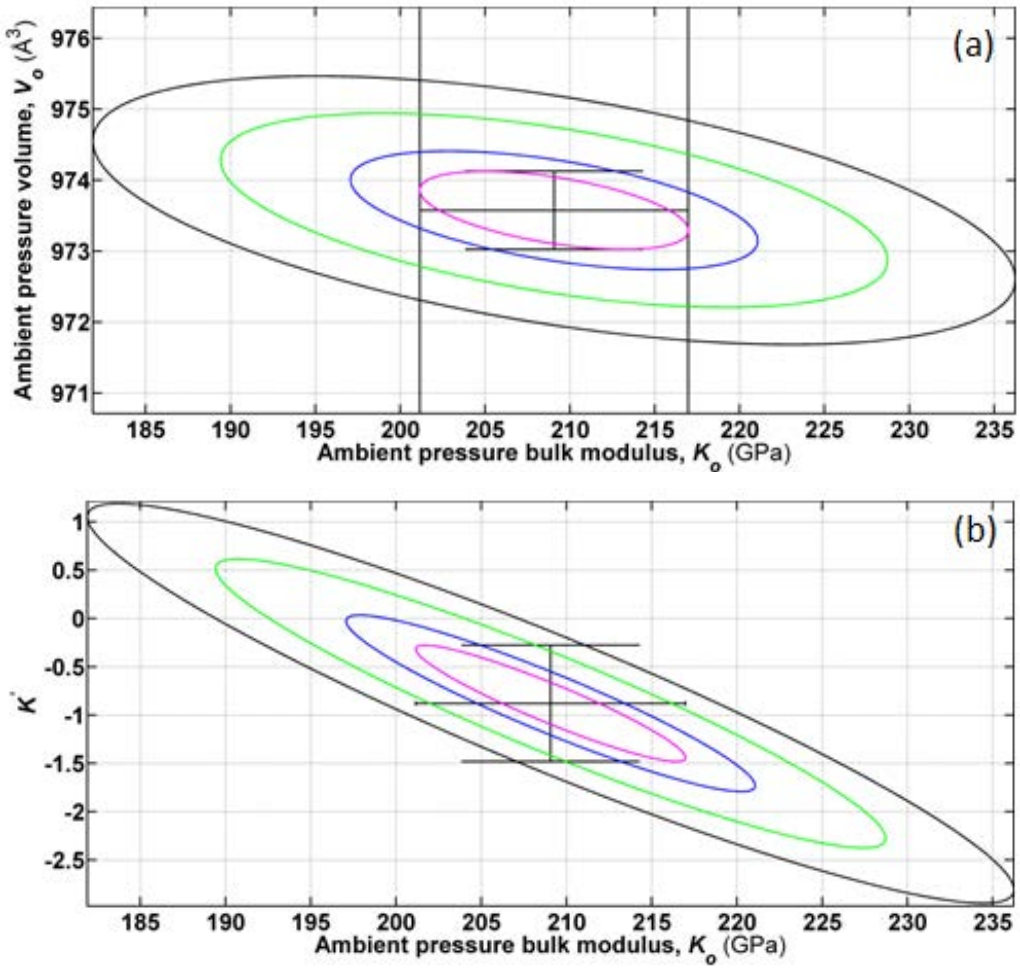

FIG. 6. Confidence ellipses from a third order Birch-Murnaghan EOS model weighted fit to Ta_2O_5 data. (a) Vo vs. Ko, and b) K' vs. Ko. The magenta colored ellipse is 0.607-σ (50.3% confidence), blue is 1-σ (68.3% confidence), green is 2-σ (95.4% confidence), and the black ellipse is 3-σ (99.7% confidence).