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An Experimental and Theoretical Multi-Mbar Study of Ti-6Al-4V

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ABSTRACT

We report results from an experimental and theoretical study of the room temperature (RT) compression of the ternary alloy Ti-6Al-4V. In this work, we have extended knowledge of the equation of state (EOS) from 40 GPa to 221 GPa, and observed a different sequence of phase transitions to that reported previously for pure Ti.

INTRODUCTION

The commercial and industrial importance of the two-phase ternary alloy Ti-6Al-4V (wt %) is well documented and known to be heavily dependent on its mechanical properties (see for example [1]). Ti-6Al-4V (hereafter referred to as Ti64) crystallizes predominantly in the two-atom α -phase (hexagonal-close-packed or hcp) at ambient conditions, with a much smaller fraction by volume crystallizing in the β -phase (body-centred-cubic or bcc) around the grain boundaries. The alloying of substitutional and interstitial impurities increases the strength of Ti64 compared with pure Ti. Al is the α -phase stabilizer and dominant substitutional strengthener.

At room temperature (RT), using diamond anvil cells (DACs) and angle-dispersive X-ray diffraction (ADXRD) [2], the α -phase of Ti64 has been observed to transform into the three-atom hexagonal ω -phase at 27 GPa. A more recent RT DAC study, using energy-dispersive X-ray diffraction (EDXRD), did not observe any phase transformation up to 32.4 GPa [3]. Shock studies of Ti64 are fairly extensive, but no evidence of a phase transformation has been observed (see for example [4] and references contained therein).

Pure Ti has been compressed at RT using DACs to 220 GPa, and the transformation sequence $\alpha \rightarrow \omega \rightarrow \gamma \rightarrow \delta$ was reported [5, 6], where the γ and δ phases are orthorhombic distortions of the hcp and bcc structures, respectively. The effects of uniaxial stress on the $\alpha \rightarrow \omega$ transition in Ti were studied by Errandonea *et al.* [7] using DACs and ADXRD. They found that the transition pressure was dependent on the pressure transmitting medium (PTM) used, and ranged from 4.9 GPa (no PTM) up to 10.5 GPa (argon PTM). In addition, they observed the coexistence of the α and ω phases over a large pressure range.

Our motivation for conducting the present study was to determine whether or not Ti64 exhibited similar behavior to that reported for pure Ti at multi-megabar pressures.

EXPERIMENT AND THEORY

Experimental details

We performed a number of static high-pressure compression experiments using gas-membrane driven DACs at the High Pressure Collaborative Access Team (HPCAT) beamline 16-IDB, at the Advanced Photon Source (APS), in Chicago. We collected ADXRD patterns from commercially-sourced Ti64 powder (Goodfellow) embedded in a variety of pressure media, and loaded into rhenium gaskets with either a Cu or a Ta pressure marker.

Initially, we studied the $\alpha \rightarrow \omega$ phase transition. In order to investigate the effects of uniaxial stress on this transition we used a variety of PTMs, and loaded samples of Ti64 into DACs with (in increasing order of hydrostaticity): no PTM; mineral oil; 4:1 methanol-ethanol; and neon. Figure 1 shows a representative stacked plot of ADXRD patterns obtained from Ti64 embedded in a neon PTM and with a Cu pressure marker. We clearly observe a coexistence of the α and ω phases over a large pressure range (between 32.7 GPa and ~ 44.4 GPa). The dominant ω (110/101) reflections first appear at ~ 32.7 GPa, and with further increases in pressure, the ω (110/101) reflections increase in intensity, the strong α (101) reflection decreases in intensity, and the weaker, ω (001) and ω (201) peaks appear. By 44.4 GPa, the α-phase peaks have almost completely disappeared. In all, we were able to index up to 11 α-phase peaks and 8 ω-phase peaks.

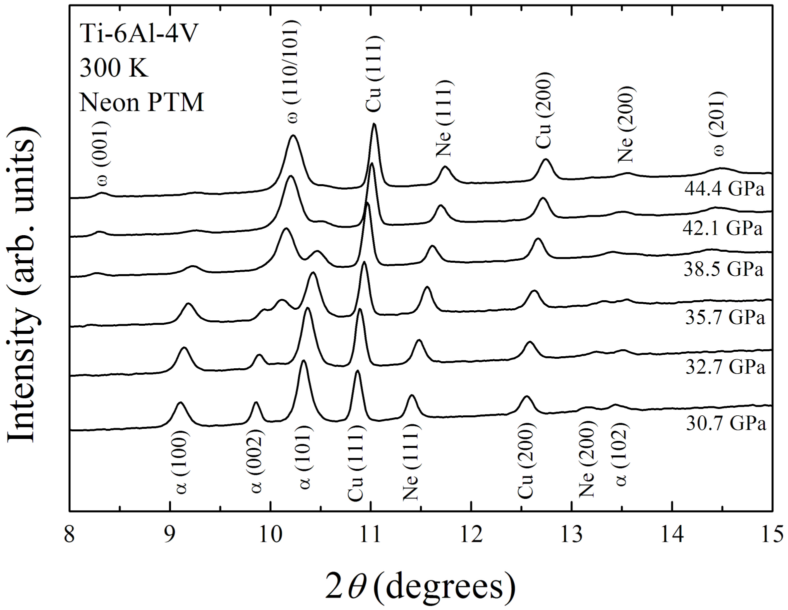

Figure 1. A stacked plot showing Ti64 ADXRD patterns collected on pressure increase from 30.7 GPa to 44.4 GPa. Diffraction peaks from the the α and ω phases, and from the Cu pressure marker and neon PTM are indexed.

We observed similar behavior in the $\alpha \rightarrow \omega$ transformation for all of the PTMs used in this study. The more hydrostatic the PTM, the higher the pressure at which the $\alpha \rightarrow \omega$ transition occurred. Table I summarizes the observed transition pressures, and the measured K_0 and K' of the α -phase in different PTMs (including previously-published observations). The α -phase data were fitted using the Vinet EOS formulation [8]. We measured the volume at ambient conditions to be V_0 = 17.252 Å^3.

Table I. Summary of the observed $\alpha \rightarrow \omega$ transformation for Ti64. The transition pressure is the first appearance of peaks from the ω phase. K_0 and K' are the bulk modulus, and its pressure derivative, of the α phase, as determined from fitting the compression data to a Vinet EOS.

Pressure medium (PTM)	$P\alpha \rightarrow \omega$ (GPa)	K_0 (GPa)	K'
No medium	26.4	100 ± 12	4.46 ± 1.50
Mineral oil	26.2	106 ± 10	5.07 ± 1.23
4:1 methanol-ethanol	31.2	115 ± 3	3.22 ± 0.22
Neon	32.7	101 ± 3	4.05 ± 0.29
4:1 methanol-ethanol [2]	27.3	125	2.41
N/A [3]	N/A	154 ± 11	5.45 ± 1.44

To search for further phase transitions at higher pressures, we compressed Ti64 in a mineral oil PTM to 221 GPa. We observed a sluggish phase transition between 95 GPa and 123 GPa to a new phase (henceforth referred to as the β phase) which had the bcc structure. Figure 2 shows integrated ADXRD patterns obtained over this pressure range, showing the gradual disappearance of the (210) and (002) reflections from the ω phase that mark this transition.

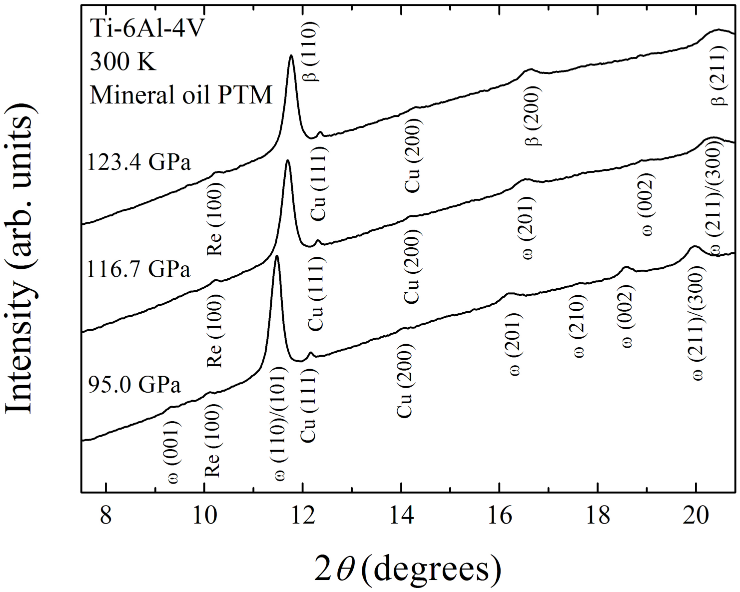

Figure 2. ADXRD patterns of the $\omega \rightarrow \beta$ phase transition for Ti64 between 95 and 123 GPa. Peaks from the ω and β phases, the Cu pressure marker and the Re gasket are indexed.

The β-phase is stable to 221 GPa, the highest pressure reached in this study, and we find no evidence of the orthorhombic γ and δ phases reported in pure Ti. The *P-V* plot of the RT compression of Ti64 in a mineral oil PTM to 221 GPa is shown in Figure 3.

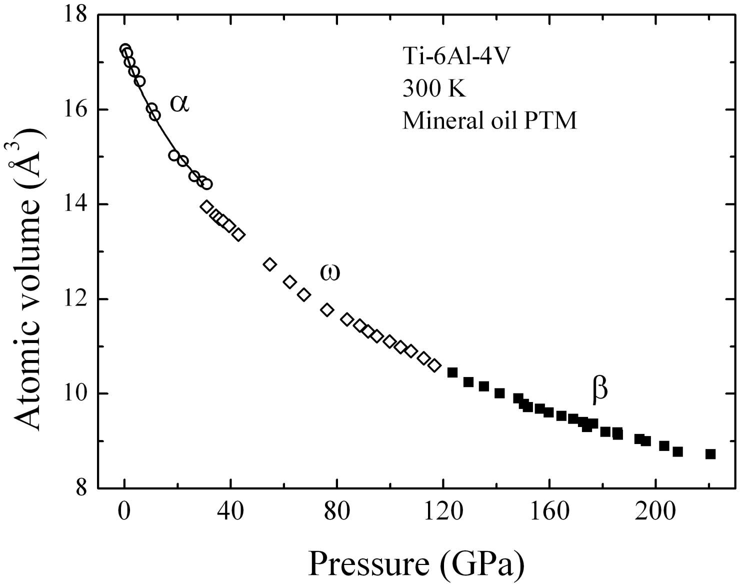

Figure 3. The change in the atomic volume and crystal structure of Ti64 with increasing pressure. The solid line shows the Vinet fit to the α-phase data.

The volume change across the $\alpha-\omega$ boundary was less than 1% for Ti64 in both a neon and 4:1 methanol-ethanol PTM. For Ti64 in mineral oil, the volume change was 2.5% and for no PTM the volume change was 4.5%. However, the Ti64 data collected using no PTM was difficult to analyze because of the presence of Re peaks in the diffraction patterns at pressures below 30 GPa. Consequently, our quoted volume change across the $\alpha-\omega$ boundary may be in error.

Theoretical Details

We performed our theoretical calculations using the plane-wave DFT-code CASTEP [9], using supercells of 54 atoms for each configuration, to get impurity levels of 2 at%. The k-point density for each configuration was 0.05 Å^{-1}. A plane-wave cut-off of 500 eV was used for basis-set convergence. In all cases, the alloy composition was 85.2 at% Ti, 11.1 at% Al and 3.7 at% V, that is, 46 atoms of Ti, 6 atoms of Al and 2 atoms of V. We chose the one that gave the lowest energy.

The calculated enthalpies of the ω and β phases, relative to that of the α-phase, (at T = 0 K) as a function of pressure are shown in Figure 4. The calculated $\alpha \rightarrow \omega$ transition pressure is

24 GPa, in agreement with our experimental data. The transition pressure to the β phase is predicted to be around 110 GPa , again in reasonable agreement with our experimental data.

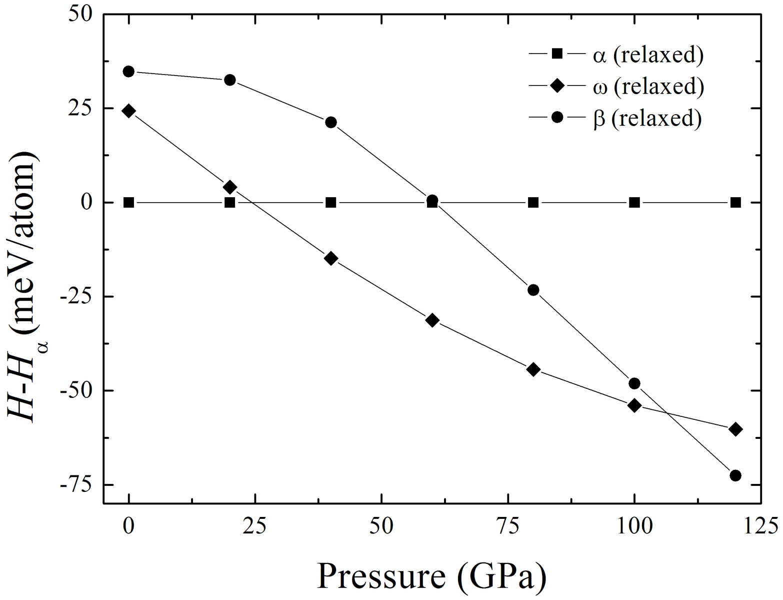

Figure 4. The calculated enthalpies of the ω and β phases, relative to that of the α -phase, as a function of increasing pressure. The transition pressures are taken from where the lower curves cross.

Above 110 GPa, our calculations found the cubic β phase to always be more stable than the orthorhombic γ and δ phases.

DISCUSSION AND CONCLUSIONS

We have performed a series of ADXRD DAC experiments to extend knowledge of the EOS of Ti64 from 40 GPa to 221 GPa. In so doing, we have confirmed the occurrence of the $\alpha \rightarrow \omega$ phase transition at a much higher pressure (26.2 GPa - 32.7 GPa) than is the case for pure Ti (4.9 GPa - 10.5 GPa). This is to be expected, as the alloying of the α -phase stabilizer (Al) suppresses the $\alpha \rightarrow \omega$ phase transition.

In contrast to a previous study [2], we observed the coexistence of the α and ω phases over a large pressure range. Errandonea *et al*. also observed such a coexistence of these phases for pure Ti [7]. Thermodynamically, it should not be possible to have a coexistence of phases over a range of hydrostatic pressures without chemical separation. However, the observation of phase coexistence is not uncommon in DAC experiments and could well be a consequence of the non-hydrostatic conditions that inevitably exist in this uniaxial pressure device, even when using a PTM such as neon.

We observed a phase transition from the ω phase to the bcc β-phase between 117 GPa and 123 GPa when using a mineral oil PTM, and found the β-phase to be stable to at least 221 GPa. This transition sequence is different to the reported for pure Ti, where there are transitions to the orthorhombic δ and γ phases [5, 6]. A possible cause of the different transition sequence found in Ti64 could be the presence of a PTM in our experiment, as opposed to the absence of a PTM in the previous Ti experiments [5, 6]. Studies of Ti to above 200 GPa using a PTM are planned. DFT calculations of the $\alpha \rightarrow \omega$ and $\omega \rightarrow \beta$ transition pressures are in good agreement with our observed values.

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