Thermal expansion and lattice parameters of shaped metal deposited Ti–6Al–4V

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ABSTRACT

Thermal expansion and lattice parameters are investigated up to 1100 °C for Ti–6Al–4V components, fabricated by shaped metal deposition. This is a novel additive layer manufacturing technique where near net-shape components are built by tungsten inert gas welding.

The as-fabricated SMD Ti–6Al–4V components exhibit a constant coefficient of thermal expansion of 1.17×10^{-5} K^{-1} during heating up to 1100 °C, not reflecting the α to β phase transformation. During cooling a stalling of the contraction is observed starting at the β transus temperature. These high temperature experiments denude the α phase of V and enrich the β phase.

The development of the lattice parameters in dependence on temperature are observed with high temperature X-ray diffraction. The unit cell volumes derived from these parameters are at room temperature larger for the α than for the β phase. With increasing temperature the unit cell volume of the β phase increases stronger than the one of the α phase resulting in a similar unit cell volume at the β transus temperature.

These observations are interpreted as an indication for as-fabricated the SMD components being in a non-equilibrium state and reaching equilibrium during the slow heating and cooling during of the two different high temperature experiments.

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1. Introduction

Titanium alloys are widely used when excellent strength to weight ratio [1], superior biocompatibility, low elastic modulus and/or enhanced corrosion resistance are needed [2]. Examples for this can be found, for example, in applications for aerospace, implants, and sports equipment [1–3]. One of the most widely applied Ti alloy is Ti–6Al–4V [3].

Ti is a costly metal and traditional machining of Ti alloys is expensive and time consuming. It is especially difficult to machine since it is prone to oxygen contamination at high temperatures. This contamination results into the formation of a brittle surface layer, the so-called α case [4,5]. In order to avoid this α case, low machining rates are required which increases the machining time and the costs.

Hence, near net-shape production by innovative manufacture routes would be of great advantage, which in addition would reduce the amount of scrap and the fabrication time to the end product. So-called additive layer manufacturing can fulfil these requirements. Several techniques are currently under investigation, where different heat sources such electron beam [6–9], laser [9–18], or a

welding torch [19–29] are applied. The later is called shaped metal deposition (SMD), a technique patented by Rolls Royce, which is the topic of the present paper.

Additive layer manufacturing allows rapid fabrication of 3D objects, layer by layer directly from a computer aided design data source. Furthermore, it is promising in small-scale production of parts and for repair of high performance alloy components. However, additive layer manufacturing in general, and therefore also SMD, exhibits a rather peculiar fabrication scheme with repeated exposure to high temperatures, thermal gradients and cooling rates. This peculiar thermal history has a major impact, since the morphology and therefore the properties of Ti alloys depend critically on it. For example, the Ti–6Al–4V equilibrium phase diagram predicts at high temperatures the body centred cubic β phase and a α + β phase field below 1000 °C (Fig. 1). When, during manufacturing, these different phase fields are traversed, different morphologies can be obtained depending on the cooling rate [30–33]. Colony structures and basket weave Widmanstätten structures with α phase lamellae in a residual β phase matrix do occur during slow or medium fast cooling rates. At very high cooling rates (>410 °C/s) diffusion based transformation to the α + β phase may be omitted and passing the MS line (Fig. 1), the result is a fully martensitic hcp α′ phase microstructure [32]. Naturally, also intermediary or mixed states may arise. Not only the morphology, but also the composition of the phases may depend on the thermal history. For example, for higher cooling rates a departure from the
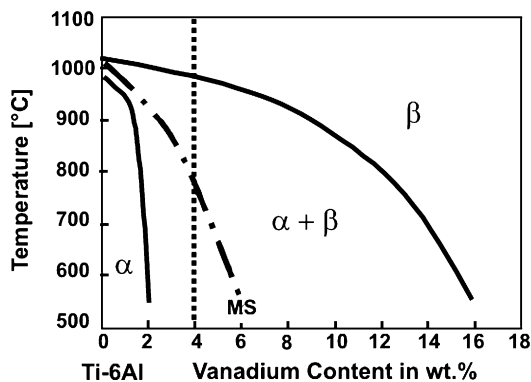
Fig. 1. Schematic ternary phase diagram Ti–6Al–V (MS: martensite start temperature) after [3]. Copyright Wiley-VCH Verlag GmbH & Co. KGaA. Reproduced with permission.

equilibrium phase boundaries can be expected, decreasing the size of the α + β phase field [34], and leading to an α phase composition higher in vanadium and poorer in aluminium than in the equilibrium case. The non-equilibrium β phase composition would then be lower in vanadium and higher in aluminium.

It has been shown elsewhere, that Ti–6Al–4V SMD components consist mainly of α lamellae in a β matrix, either colony or basket weave Widmanstätten, with no indication for the martensitic α′ phase [25,26]. Furthermore, it has been demonstrated, that this material is highly textured, and that the β to α transformation obeys the Burgers orientation relationship [25]. This microstructure differs significantly from the one in material fabricated by conventional techniques, and the properties can therefore not necessarily be simply deduced. The goal of the present paper is to investigate the thermal expansion and relate it with the lattice parameters measured by X-ray diffraction (XRD).

2. Experimental

2.1. Shaped metal deposition

The SMD cell consists of a tungsten inert gas (TIG) welding head, attached to a 6-axis Kuka robot linked to a 2-axis table, all of which are enclosed in an airtight chamber. The setup is located at the AMRC, Sheffield, United Kingdom. In the present case, a Ti–6Al–4V grade 5 wire with a diameter of 1.2 mm in an inert argon atmosphere (99.999% purity) is applied to build a component. Layer by layer, with rotating the table to keep a constant torch direction, a tubular shape with squared cross-section (0.15 m × 0.15 m), a height of 0.12 m, and a wall width of 0.01 m was built. The controlled parameters were the wire feed speed of 2.4 m/min, the table speed of 0.3 m/min and the electrical current of 150 A.

2.2. Thermal mechanical analysis

The thermal expansion in dependence on the temperature has been measured by the Netzsch DIL 402C dilatometer, a set-up also called TMA (thermo-mechanical analysis), in vacuum up to 1100 °C with a heating and cooling rate of 2 °C/min. Generally, before starting the TMA the vacuum chamber was flushed three times with argon and evacuated. In one case, the chamber was pumped after the third flushing for a whole day resulting in a better vacuum than in the case of starting the test after pumping for 1 h after the third flushing.

2.3. X-ray diffraction including high temperature measurements

The room temperature X-ray diffraction (XRD, 3003-TT, Seifert, Ahrensburg, Germany) was carried out in ambient atmosphere. The high temperature diffraction experiments (HT-XRD) were performed with the same diffractograph in continuous flow of Ar applying in addition a high temperature furnace (HDK 2.4 X-ray furnace, Johanna Otto, Hechingen, Germany). The testing temperatures were 50 °C and further from 300 up to 1100 °C increasing in 200 °C steps. The same temperatures were investigated during cooling down. The room temperature XRD was performed in the 2Θ range from 20° to 120° with a step size of 0.02° and a scan step time of 2 s. The HT-XRD was performed in the 2Θ range from 30° to 95° with a step size of 0.05° and a scan step time of 1 s.

As already mentioned, the Ti–6Al–4V SMD components are highly textured and in some sense can be considered as pseudo-single-crystalline [25]. The diffraction

pattern of such highly textured component depends critically on the orientation of the component relative to the X-ray beam and frequently the required Bragg condition is not accomplished. Hence, the appearance and the height of diffraction peaks usually do not agree with the one derived from powders. A consequence of this is that the relative amount of two phases cannot be derived from the relative intensities. Yet, if a diffraction peak appears, the diffraction angle 2Θ can be used, applying Bragg's law, to determine the distance of the reflecting planes *d*. With the reflecting planes the lattice parameter can be derived. For hexagonal closed packaged structures, such as the α phase, the lattice parameters *a* and *c* can, for example, be calculated using the [100], [110], [002], and [102] reflections:

$$a = d_{100} \frac{2}{\sqrt{3}} \tag{1}$$

$$a = 2d_{110} \tag{2}$$

$$c = 2d_{002} \tag{3}$$

$$c = \frac{2}{\sqrt{(1/d_{102}^2) - (4/3)(1/d_{110}^2)}} \tag{4}$$

For bbc structures, such as the β phase, the lattice parameter *c* can be derived by:

$$c = 2d_{200} \tag{5}$$

The unit cell volume *V* then is

$$V_\alpha = \frac{\sqrt{3}}{2} ca^2 \quad \text{or} \quad V_\beta = c^3 \tag{6}$$

The average length *L* for the unit cell, which will be taken as a measure for length changes, can be approximated by

$$L = \sqrt[3]{V} \tag{7}$$

2.4. Scanning electron microscopy including EDX

The microstructure was investigated by scanning electron microscopy (SEM, FEI XL30FEG) of polished cross-sections, where back-scattered electron (BSE) imaging with very high contrast allows discerning directly the α and β phases, omitting artefacts from etching. Energy dispersive X-ray (EDX) point analysis was applied to determine the composition of the phases.

2.5. Micro-Vickers hardness

The Vickers microhardness tests were performed on polished cross-sections of as-fabricated specimens and of specimens tested by IET or TMA applying a Leitz/Durimet 2 microhardness tester using a weight of 100 g (HV0.1).

3. Results

3.1. Thermal mechanical analysis

During heating in a good vacuum the SMD specimen exhibits continuous linear expansion until 1100 °C, not exhibiting any variation while passing the α + β phase field or reaching the β phase field (Fig. 2(a)). Hence, in the case of as-fabricated material, phase transformations are not reflected in the TMA. The coefficient of thermal expansion (CTE) during heating is $1.17 \times 10^{-5} \, K^{-1}$. During cooling, first the contraction line follows the expansion line until reaching the β transus temperature at 1000 °C. Then, the contraction stalls until about 900 °C. Further on, again linear contraction is observed with a slope similar to the expansion. The stalling during heating between 1000 and 800 °C results into a hysteresis and a net-increase of the specimen length of about 0.1%.

The experiment in the poorer vacuum shows the influence of oxygen (Fig. 2(b)). During heating, until about 800 °C a similar CTE as in the case of the good vacuum is observed. At higher temperatures, however, increased expansion is recorded. Also, during cooling, in the regime between 1100 and 1000 °C, the contraction rate is slightly lower than the observed expansion rate during heating. Therefore, due to the poorer vacuum the hysteresis is opened up more and a net-increase of the specimen length of about 0.2% is observed. However, the general result in both cases is the same: during heating the phase transformation from α to β is not reflected in the TMA curve, while during cooling the transformation from β to α phase results in an increased length.