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EVOLUTION OF MICROSTRUCTURE DURING SHAPED METAL DEPOSITION

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Abstract. In a companion paper, the correlation between the temperature field and the microstructure has been studied in a series of specimens made by Shaped Metal Deposition (SMD). The aim of the present paper is to improve the microstructure evolution model by taking into account not only the temperature and its rate but also the kinetics of the different solid phase transformations occurring in the Ti-6Al-4V alloy along the multiple heating and cooling cycles. At high temperature (above the beta-transus ~1000°C), Ti-6Al-4V is in the beta phase field. During cooling, the beta phase may transform to martensitic or massive alpha, Widmanstätten alpha or grain-boundary or colony alpha, depending on the cooling rate. Transformation to martensitic/massive alpha takes place under rapid cooling and is assumed to be diffusionless or instantaneous. At lower cooling rates, Widmanstätten and grain boundary/colony alpha growth is diffusion-controlled. Further, the diffusive transformation of martensitic/massive alpha into Widmanstätten alpha is considered during cooling based on observations. In addition, during heating, diffusion-controlled transformation of martensitic/massive alpha into Widmanstätten alpha and instantaneous growth of the beta phase fraction at the expenses of the fractions of martensitic/massive alpha, Widmanstätten alpha, and grain-boundary/colony alpha is assumed.

For diffusive transformation, the temperature history of a point (computed as described in the companion paper) is approximated as a series of isothermal steps where the transformation is governed by the Johnson-Mehl-Avrami law. Massive/martensitic transformation is described using the Koistinen-Marburger law, while transformation of martensitic/massive alpha, Widmanstätten alpha, and grain-boundary/colony alpha into beta during heating is assumed to follow the beta equilibrium curve.

Numerical results are compared to the experimentally observed microstructure, which helps to understand the complex transformation modes taking place during the repeated heating and cooling sequences of a SMD run.

1 INTRODUCTION

Shaped Metal Deposition (SMD) is a novel rapid prototyping technique to build near-net shape metal pieces layer by layer, which allows avoiding time and material intensive machining. The SMD rig consists of a welding robot with a Tungsten Inert Gas (TIG) torch housed in an argon filled chamber and the material is supplied by wire which is fed into the chamber through an annular feed pipe. The robot follows a computer aided design (CAD) code in order to make the desired piece by the deposition of successive weld layers.

During SMD, each material point in the deposited wall is subjected to repeated heating and cooling cycles, which determines the microstructure around it. The thermal history at each point determines the evolution of the microstructure at this location. Generally, the microstructure of SMD components made by Ti-6Al-4V mainly consists of α phase lamellae embedded in residual β phase (Baufeld et al., 2009). In more detail, the top 1 cm region of the components exhibit very fine lamellae, while the components below this top region consist of coarser lamellae. This top region has been attributed to the area subjected to temperatures above the β-transus during the last deposition step (Baufeld et al., 2009). Furthermore, the bottom region displays a banded structure parallel to the base plate, representing, according to Baufeld et al. (2009) the β-transus lines of preceding deposition steps.

In order to support these explanations, detailed modelling of the thermal history and the resulting phase transformations are required. Earlier work by Charles and Järvstråt (2009) can be taken as starting point. However, the modeling results have contradicted severely their own experimental results. Specifically, the model predicts a large amount of martensitic phase in the top region, which, according to their experimental observation, consists mainly of a Widmanstätten microstructure. Therefore, the model needed improvement by considering additional possible phase transformations. The present paper is based on a model for the thermal analysis of SMD processes (Fachinotti et al., 2010), with the aim to develop the coupling of this thermal model with evolution laws for the different solid phases of Ti-6Al-4V alloys.

2 MICROSTRUCTURE MODELLING

This work is focused in the prediction of the microstructure in square tubes made by SMD of Ti-6Al-4V, like that shown in Figure 1.

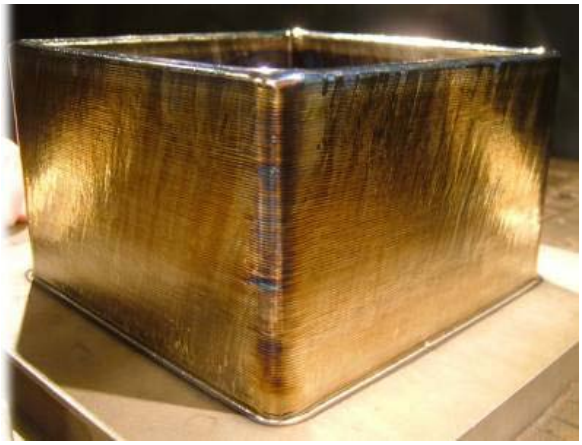

Figure 1: Square cylinder produced by SMD.

The thermal analysis of this process was described in a companion paper (Fachinotti at al, 2010). Figure 2 shows some results obtained using this model, particularly the temperature

history at some points of the so-called sample 22, made of Ti-6Al-4V using the SMD settings listed in Table 1.

Thickness	Side length	Total height	Number of layers	Current	Voltage	Wire feed rate	Welding velocity
9.49 mm	140 mm	70 mm	87	164.7 A	11.2 V	1400 mm/min	250 mm/min

Table 1: Geometrical data and process parameters used to build the sample 22.

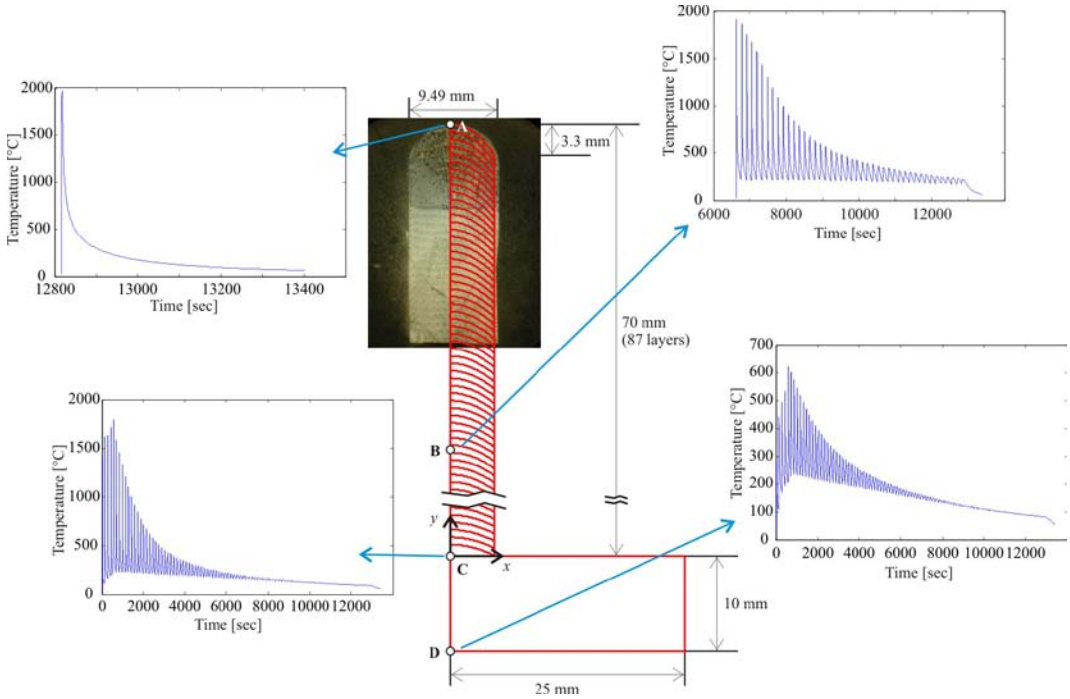

Figure 2: Temperature evolution at points A(0, 70 mm), B(0, 35 mm), C(0, 0) and D(-10 mm, 0).

In the following the focus is on the modeling of the evolution of the microstructure during the fabrication of one of this sample.

Up-to-date, the most complete model for the evolution of microstructure in Ti-6Al-4V has been proposed by Charles and Järvstråt (2009). The transformations they considered are listed in blue in Table 2. However, some improvements are needed to match some observations made in multi-pass welding and particularly in SMD of Ti-6Al-4V.

First, according to Charles and Järvstråt (2009), martensite or massive α_m only transforms to Widmanstätten α during heating, and it does this via a diffusive mechanism whose kinetics is defined using parameters taken from Gil Mur et al. (1996). Applying this model under the rapid heating conditions met in the heat affected zone (HAZ), a high fraction of α_m remains at high temperatures, where, however, the absence of α_m is widely accepted. Charles and Järvstråt (2009) made up this deficiency of the diffusive model by forcing α_m to disappear at 800°C during heating, even if α_m was still high just below this temperature. Instead of imposing this unphysical jump in the fraction of α_m at 800°C, the complete decomposition of α_m during rapid heating suggests that an instantaneous transformation should also take place.

Further, according to Gil Mur et al. (1996), α_m decomposes not only to α_W but also to β. This latter transformation is ignored by Charles and Järvstråt (2009).

On the light of these observations, we propose to improve Charles and Järvstråt's model by including an instantaneous transformation of α_{m} into β, which is assumed to be analogous to that of α_{gb} and α_{W} into β.

Furthermore, in samples taken from SMD, Baufeld et al. (2009) have observed microstructures in the top region consisting of α llamellae in a β matrix, which was interpreted to be formed via diffusive mechanisms. Due to the high cooling rates developed within this region just below the β-transus, α_{m} should form there at the beginning of cooling according to Ahmed and Rack (1998).However, the observations of Baufeld et al. (2009) suggest the development of an ageing process responsible for the decomposition of α_{m}, as reported by Qazi et al. (2003) for hydrogenated Ti-6Al-4V. This transformation is assumed to be analogous to the diffusive transformation $\alpha_{\mathrm{m}} \rightarrow \alpha_{\mathrm{W}}$ developed under slow heating.

As a summary, Table 2 depicts in red the modifications currently introduced to Charles and Järvstråt's model for a better representation of the evolution of the microstructure in SMD of Ti-6Al-4V.

Transformation	Cooling	Heating
Diffusive	$\beta \rightarrow \alpha_{\mathrm{W}}$ $\beta \rightarrow \alpha_{\mathrm{gb}}$ $\alpha_{\mathrm{m}} \rightarrow \alpha_{\mathrm{W}}$	$\alpha_{\mathrm{m}} \rightarrow \alpha_{\mathrm{W}}$
Diffusionless	$\beta \Rightarrow \alpha_{\mathrm{m}}$	$\alpha_{\mathrm{w}} + \alpha_{\mathrm{gb}} + \alpha_{\mathrm{m}} \Rightarrow \beta$

Table 2: Diffusive (→) and diffusionless (⇒) solid-phase transformations in Ti-6Al-4V. In blue: transformations considered by Charles and Järvstråt (2009), in red: current modifications.

2.1 Diffusive transformations

The diffusive transformation of the parent phase M into the product phase P that occurs at constant temperature T is usually described using the Johnson-Mehl-Avrami-Kolmogorov (JMAK) law:

$$f_P(t,T) = \left[1 - \exp\left(-k_{M\rightarrow P}(T)t^{n_{M\rightarrow P}(T)}\right)\right] f_P^{eq}(T) \tag{1}$$

where f_P is the fraction of the product phase at time t, f_P^{eq} is the equilibrium fraction of the product phase, and $k_{M\rightarrow P}$ and $n_{M\rightarrow P}$ are the thermo-dependent parameters that define the kinetics of the $M \rightarrow P$ transformation, that can be computed from the TTT curves for this transformation. In this work, and following Charles and Järvstråt (2009), the parameters for $\beta \rightarrow \alpha_{\mathrm{gb}}$ and $\beta \rightarrow \alpha_{\mathrm{W}}$ transformations were taken from Malinov et al. (2001), and those for the $\alpha_{\mathrm{m}} \rightarrow \alpha_{\mathrm{W}}$ transformation were taken from Gil Mur et al. (1996).

According to the Scheil's additivity rule (Lusk and Jou, 1997), any arbitrary temperature history can be approximated as a series of isothermal steps. Once the fraction $\mathrm{f_P(t_0, T_0)}$ of the product phase at the instant $\mathrm{t_0}$ (when the temperature is $\mathrm{T_0}$) is known, the fraction at $\mathrm{t_1 = t_0 + \Delta t}$ (when the temperature is $\mathrm{T_1}$) is computed as follows:

$$f_P(t_1,T_1) = \left[1 - \exp\left(-k_{M\rightarrow P}(T_1)(t_0^* + \Delta t)^{n_{M\rightarrow P}(T_1)}\right)\right] f_P^{eq}(T_1) \tag{2}$$

where t_0^* is the time needed to obtain $f_P(t_0,T_0)$ during an isothermal transformation at temperature T_1:

$$t_0^* = \left[\frac{1}{k_{M\to P}(T_1)} \ln \frac{f_P^{eq}(T_1)}{f_P^{eq}(T_1) - f_P(t_0, T_0)}\right]^{\frac{1}{n_{M\to P}(T_1)}} \tag{3}$$

It is worthwhile to note that this approach gives an additional, theoretical support to the use of the law describing the $\alpha_{\mathrm{m}} \to \alpha_{\mathrm{W}}$ transformation for heating as well as for cooling.

2.2 Diffusionless transformations

2.2.1 Martensitic transformation

There is no general agreement about the nature of massive transformation in Ti-6Al-4V. While some authors (Ahmed and Rack, 1998; Kleinschmidt et al., 2005) consider massive α formed by a diffusion-controlled mechanism, others authors (Kelly, 2002; Lütjering and Williams, 2007) considers it a martensitic morphology, also known as lath or packet martensite. In any case, it is accepted that massive α forms for relatively high cooling rates (between 20 and 410°C/sec according to Ahmed and Rack, 1997). As a first approach, α_{m} is assumed to embody (acicular) martensite as well as massive α (or lath martensite), and the $\beta \Rightarrow \alpha_{\mathrm{m}}$ transformation is assumed to be of the martensitic type. Martensitic transformations are usually defined by the Koistinen-Marburger law:

$$f_{\alpha_{\mathrm{m}}}(t,T) = \left[1 - \exp\left(-k_{\beta\Rightarrow\alpha_{\mathrm{m}}}(T - M_s)\right)\right] f_\beta(t,T) \tag{4}$$

where $f_{\alpha_{\mathrm{m}}}$ is the fraction of α_{m}, f_β is the fraction of β, and $k_{\beta\Rightarrow\alpha_{\mathrm{m}}} = 0.003$ was taken from Fan et al. (2005).

It is important to note that, citing Ahmed and Rack (1998), Fan et al. (2005) and Charles and Järvstråt (2009) assume that martensite only forms for cooling rates greater than 410°C/sec, which is actually the range for the complete transformation of β into martensite, but between 20 and 410°C/sec partial transformation can occur.

2.2.2 Instantaneous transformation to β during heating

Charles and Järvstråt (2009) assume that β reaches its equilibrium fraction instantaneously during heating, i.e.:

$$f_\beta(t_1, T_1) = f_\beta^{eq}(T_1) \tag{5}$$

They further assume that β grows at the expenses of α_{gb} and α_{W}. As explained above, α_{m} is added as a parent phase for a better description of its decomposition during rapid heating. Thus:

$$\Delta\beta = f_\beta^{eq}(T_1) - f_\beta(t_0, T_0) = -\left(\Delta\alpha_{\mathrm{W}} + \Delta\alpha_{\mathrm{gb}} + \Delta\alpha_{\mathrm{m}}\right) \tag{6}$$

Since there is no experimental nor theoretical evidence to determine in which proportion α_{W}, α_{gb} and α_{m} contribute to the growth of β, and until further experiments are conducted, the contribution of each morphology will be assumed to be proportional to the available fraction of this morphology, i.e.

$$\Delta\alpha_{\mathrm{W}} = -\frac{\alpha_{\mathrm{W}}(t_0,T_0)}{\alpha_{\mathrm{W}}(t_0,T_0)+\alpha_{\mathrm{gb}}(t_0,T_0)+\alpha_{\mathrm{m}}(t_0,T_0)}\,\Delta\beta$$
$$\Delta\alpha_{\mathrm{gb}} = -\frac{\alpha_{\mathrm{gb}}(t_0,T_0)}{\alpha_{\mathrm{W}}(t_0,T_0)+\alpha_{\mathrm{gb}}(t_0,T_0)+\alpha_{\mathrm{m}}(t_0,T_0)}\,\Delta\beta \qquad (7)$$
$$\Delta\alpha_{\mathrm{m}} = -\frac{\alpha_{\mathrm{m}}(t_0,T_0)}{\alpha_{\mathrm{W}}(t_0,T_0)+\alpha_{\mathrm{gb}}(t_0,T_0)+\alpha_{\mathrm{m}}(t_0,T_0)}\,\Delta\beta$$

3 RESULTS

Figure 3 shows the evolution of the microstructure at the point A located at the top of the wall (see Figure 2), as computed using Charles and Järvstråt's model (2009) and the current model. According to Charles and Järvstråt's model, around this point, i.e. in the top region, a large fraction of martensitic or massive α (~45%) remains at the end of the process, and it is slightly larger than the final fraction of α_{W}. This is in contradiction with experimental results by Baufeld et al. (2009) and also by Charles and Järvstråt (2009), who found α_{W} to be predominant in the top region of Ti-6Al-4V parts made by SMD. By allowing the decomposition of α_{m} into α_{W}, the current model predicts a high fraction of α_{W} at this point at the end of the process, in agreement with the experimental observations.

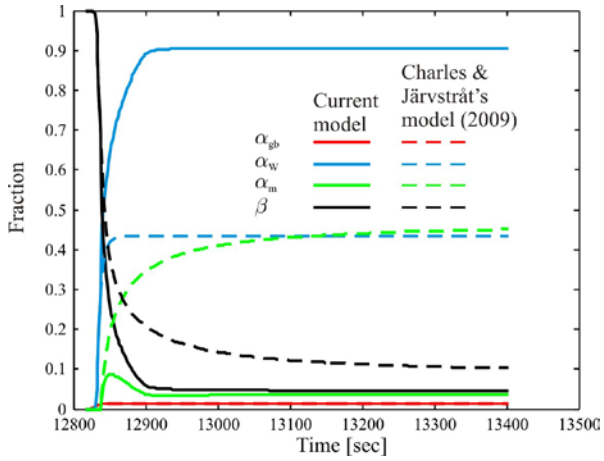

Figure 3: Evolution of microstructure at top point A(0, 70 mm).

Figure 4 summarizes the results of the improved model for the cross section of sample 22. Clearly the top and bottom region can be discerned. The top region consists mainly of Widmanstätten α phase (a fraction of 0.91), which is in agreement with the experimental findings (Baufeld et al., 2009). In addition, some massive or martensitic α, grain boundary α and β phase, all with a fraction in the order of 0.05, are predicted. The amount of the minority phases are difficult to determine, especially since grain boundary, massive and martensitic α in small quantities can not be discerned easily by conventional methods. Only the presence of β was proven experimentally.

According to the current model the bottom part contains less Widmanstätten α (~0.7) and massive or martensitic α (~0), and more grain boundary α (~0.04) and β (~0.25) than the top region. This phase distribution extends into the base plate as HAV.

The experimentally observed banded structure (left side of Figure 5) also appears in the result of the current model (right side of Figure 5). Experiment and model agree very well. Apparently, the bands are a result of variations in Widmanstätten α, grain boundary α and β.

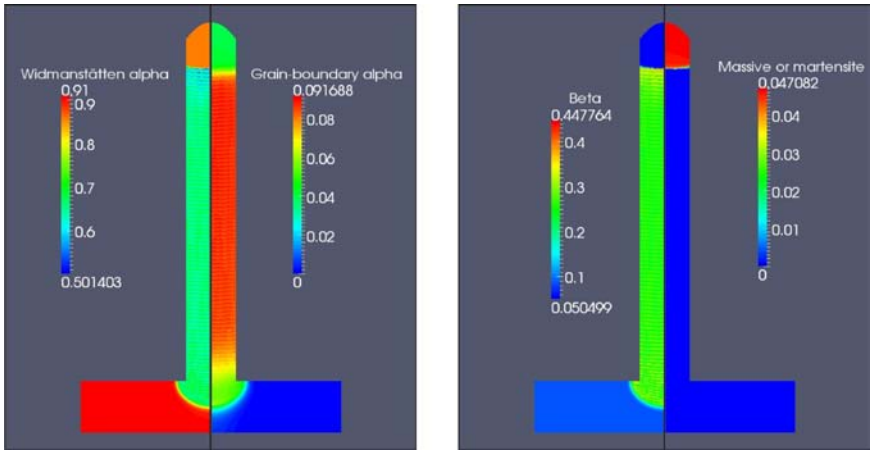

Figure 4: Final microstructure distribution in the cross section of sample 22 as computed using the current model.

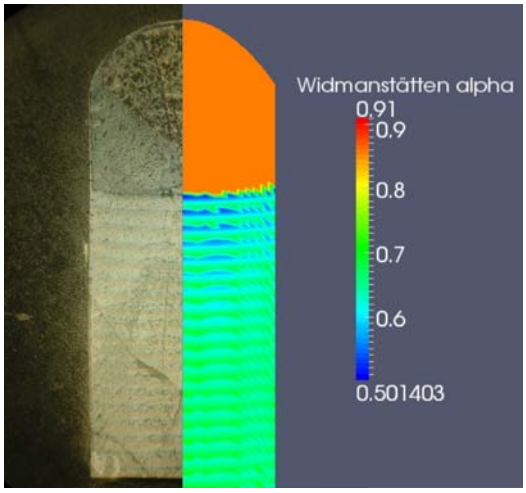

Figure 5: Final distribution of Widmanstätten $\boldsymbol{\alpha}$ in the cross section of sample 22 vs. the corresponding optical macrograph.

4 CONCLUSIONS

This work contributes to the knowledge of the complex microstructural changes that take place in Ti-6Al-4V alloy during the Shaped Metal Deposition process. Starting from the most sophisticated model available in literature (Charles and Järvstråt, 2009), improvements were proposed on the base of experimental observations. Modifications mainly concern the transformations suffered by martensitic or massive α during the multiple heating-cooling cycles the piece undergoes during the layer-by-layer deposition.

Thanks to the current improvements, a very good agreement between numerical results and with experiments is achieved.

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