Simulation for Additive Manufacturing
11th –13th October 2017
Munich, Germany

Modeling of Microstructure evolution in Additive Manufacturing processes of Ti6Al4V

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Key Words: *Additive Manufacturing, Metal deposition, Process simulation, Thermal Modeling, Microstructure Modeling,* Ti6Al4V

During iterative metal depositions, alloys experience thermal cycles characterized by an unusual range of cooling and heating conditions, if compared with traditional forming processes. The complex temperature evolution influences directly the kinetics of microstructure formations during solidification and solid state transformation. This leads to unique microstructural and mechanical properties that are distinct from cast or wrought parts obtained from identical alloys [1].
Accurate data of temperature evolution during the process are strictly needed in order to provide the thermal inputs for the modeling of microstructure formation in each point of the part. At CIMNE, several activities of thermal simulations of AM processes have been successfully carried out using COMET, a self-developed Finite Element (FE)-based framework for the solution of engineering problems [2, 3]. In these cases, a thermal solution that includes phase-change phenomena was adopted. The welding path was modeled by means of an ad-hoc activation methodology that switched on the elements according to the scanning sequence. The aim of this work is to enhance the tools of AM process simulation available at CIMNE, focusing on the implementation of models for microstructure evolution of Ti6Al4V.
A review of the state-of-the-art has been carried out in order to define which microstructural transformations take place during AM processes of a Ti6Al4V alloy and which are the most suitable models for the description of each transformation. During a general cooling, three different main transformations can take place: solidification of β phase from liquid, $\beta \rightarrow \alpha+\beta$ solid state transformation and α_m martensite formation. Below liquidus temperature, β phase (BCC crystal structure) starts to form. Depending on the cooling conditions, β grains can show equiaxed or columnar morphologies [4]. Following the cooling path, when the β-transus temperature (around 995 °C) is reached, α phase (HCP crystal structure) starts to form from the previous β phase. Generally, slow cooling rates lead to Widmanstätten structures, composed by α lamellae, with small amount of intra-lamellar retained β. The $\beta \rightarrow \alpha+\beta$ diffusion-controlled transformation can be modeled by means of a Johnson-Mehl-Avrami-Kolgorov (JMAK) equation [5] using the principle of the additivity rule [6]. JMAK equations are defined by temperature-dependent parameters that can be inversely extracted from literature data of Temperature-Time-Transformation (TTT) curves. α lamellae are usually aligned to form colonies and the α lath thickness, inversely proportional to cooling rate, can be modeled by an empirical Arrhenius equation. In case of faster cooling rates, martensite α_m (a non-equilibrium phase with acicular shape) can form from the residual β. This transformation is considered diffusionless and can be modeled using the Koistinen-Marburger law, an empirical relationship dependent from the undercooling below the martensite start temperature T_{ms} [7]. In the case of re-heating, three different main transformations can occur: decomposition of α_m to $\alpha+\beta$, dissolution of α to β and remelting of β. Gil Mur [8] proposed to model the $\alpha_m \rightarrow \alpha+\beta$ transformation with JMAK equations using experimental parameters extracted from martensitic samples reheating

data. Considering the high heating rates of AM processes, α→β transformation can be approximated (as the re-melting of β) as an instantaneous transformation which follows the equilibrium phase diagram [9]. However, other approaches to β recovery have been adopted in literature, such as the additivity rule with JMAK equations or the model proposed by Kelly [10], a time dependent parabolic law multiplied by a calibrated function of temperature.
The previous exposed models have been implemented in a routine, similar to the one presented in ref [11], allowing to switch from a transformation to another and to consider previous incomplete transformations. The validation of the microstructural models has been performed comparing the simulations results with data available in the literature. For some specific transformations, the outcome obtained using different models are discussed. Considerations about the sensitivity of the overall model to the variation of material parameters are also presented. Due to the high dependence from experimental parameters, future activities of material characterization could sensibly improve the accuracy of these microstructural models.

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