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De Baere, David; Valente, Emilie Hørdum; Mohanty, Sankhya; Hattel, Jesper Henry

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Modelling of the microstructural evolution of Ti6Al4V parts produced by selective laser melting during heat treatment

David De Baere[1], Emilie Hørdum Valente[1], Sankhya Mohanty[1], Jesper Henry Hattel[1]

[1]*Department of Mechanical Engineering, Technical University of Denmark*

ddbae@mek.dtu.dk

Abstract

The microstructure of parts produced by sective laser melting of Ti-6Al-4V is typically martensite in elongated prior β grains, which leads to anisotropic mechanical properties. A heat treatment can reduce this anisotropy by making these grains more equiaxed. In this work, simulations are performed wherein the evolution of the microstructure during a heat treatment is modelled using a cellular automata method. The results obtained from this simulation are compared to experimentally obtained micrographs. The simulated microstructure shows a similar evolution of the prior β grains from columnar to equiaxed, although the average diameter of the grains is slightly smaller in the simulations.

Microstructural modelling, Cellular Automata, Ti-6Al-4V, Selective laser melting, Heat Treatment

1. Introduction

Additive manufacturing allows the production of parts with very complex geometry or in small production volumes [1], with limited to no cost for developing new jigs & fixtures. One of these production techniques is selective laser melting (SLM). In this powder bed-based process, a layer of powder is deposited, and locally melted in the desired shape. The process is repeated for the next layers until the part is completed. As a consequence of this production technique, the microstructure, and thus the properties of the material, are anisotropic. The grain morphology of parts produced by SLM is typically columnar [2–5]. A predominantly columnar microstructure can be detrimental for most applications as isotropic mechanical properties are usually desired; but a proper heat treatment can offer a solution. In the material under investigation, namely Ti-6Al-4V, the columnar grains are entirely comprised of hexagonal martensite (α') [3,4]. Heating the part above the β-transus, approximately 1253 K for Ti-6Al-4V [6], triggers a phase change from a HCP to BCC phase (β). As a consequence of this transformation, the prior β grains become more equiaxed [2]. During cooling a second phase change occurs inside the formed β grains, creating widmanstätten α/β at furnace and air cooling and α´martensite with quenching [7]. The equiaxed microstructure is still present after cooling down from the heat-treating temperature, and consequently changes the mechanical properties of the part. In this paper, the microstructural evolution from columnar α' to equiaxed β at elevated temperatures is modelled to gain insight in the mechanisms behind this change, which will allow to predict the change in properties and residual stresses in future work, thus enabling greater dimensional accuracy and first-time right production with respect to the designed part.

There are several methods available to model the microstructure, but currently three of them are used most often in metal additive manufacturing literature: kinetic Monte Carlo, cellular automata (CA) and phase field method [8]. CA is used in this paper due to its relative simplicity for implementation and easy coupling with thermal models [8]. Recently, the CA method has been used to model the growth of microstructure during primary SLM production [5,9]. However, implementations of a CA for the microstructural evolution during the heat treatment of parts produced using SLM are still scarce. The first section of this extended abstract explains how the initial microstructure for the simulations is extracted from the experimentally obtained micrographs, and is followed by a brief description of the implemented CA method. The final section documents preliminary results showing an agreement between the simulations and the micrographs of the microstructure after the heat treatment.

2. Materials and method

For validation of the developed model, micrographs of as-built and heat treated parts produced using SLM are used in this work. For the heat treatment, the samples were heated to a temperature of 1323 K for two hours in a furnace with a flow of argon, and cooled at 1.5 K/s.

2.1. Experimental results

Small Ti-6Al-4V cuboids produced using SLM were cut perpendicular to the scanning direction and the cross-section was ground, polished and etched with oxalic tinting reagent. Images of the microstructure were obtained using an OLYMPUS GX41 light optical microscope.

2.2. Image analysis

The analysis of the image is a four step process. First the images are converted into a black-and-white intensity image. Next they are divided into supercells. The intensity value of these supercells is the average of the intensity of the different pixels which make up the cell. Finally, the supercells are aggregated into grains by comparing their intensities. If the difference is low, two supercells are assumed to be in the same grain. The result is shown in **figure 1**. Next, the average line diameter of the grains is extracted from this image, and used as input to generate an idealised microstructure for further modelling. This idealised microstructure is shown in **figure 2 (b).**

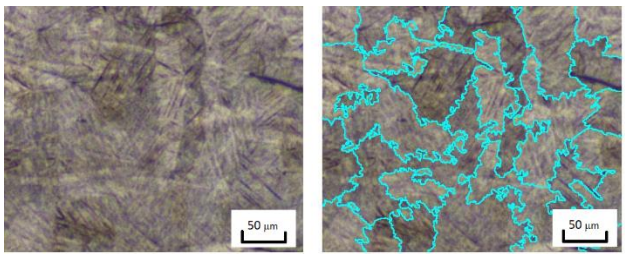

Figure 1. Original micrograph of Ti6Al4V part (left) used for identification of grain boundaries through image analysis (right).

3. Cellular Automata

This work uses a CA method to model the microstructure, based on the models developed by Rappaz and Gandin [10]. The computational domain is divided into a number of square cells, and all the cells are initiated with state ¨0¨ (original α'). In the nucleation step a number of cells change into state ¨1¨(growing). Typically for a CA, the state of a cell is determined by its neighbours. Practically this means that a cell with state ¨0¨ will transform into the growing state if any of the neighbours in the Neumann neighbourhood has a state ¨1¨. Finally, when all neighbouring cells are captured, the centre cell transforms into a state ¨2¨(transformed to β).

4. Results and discussion

Using the CA method, the microstructure after the heat treatment is predicted. The results of the simulations before and after the heat treatment are compared qualitatively in **figure 2**. Although the precise location of the grains is different due to the random position of the nucleating grains, the resultant grains are larger after heat treatment, and more equiaxed, as also observed in the experimental results. To achieve more quantitative and statistically viable results, the simulations are repeated multiple times with different nucleation points.

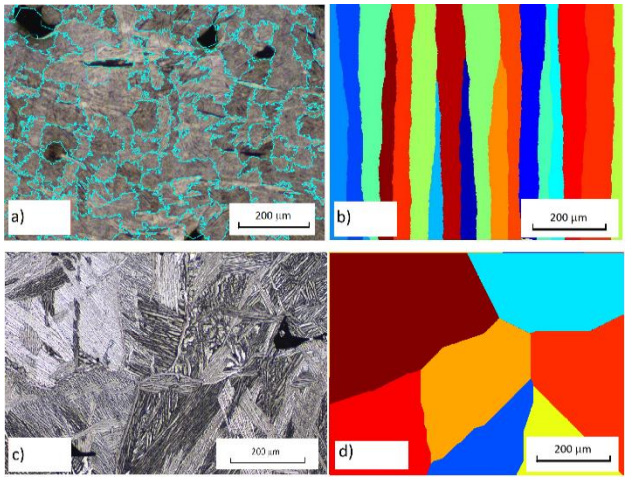

Figure 2. Original micrographs before (a) and after (c) the heat treatment, and respective modelled counterparts (b and d).

Histograms of the line diameters of the measured and the simulated microstructures are given in **figure 3**. The line diameters from both experiments and simulations can be observed to follow a similar lognormal distribution. The mean diameter from the simulations falls within the confidence interval of the experimental mean, therefore it can be concluded that the simulations manage to capture the experimental results. **Figure 3** also shows the cumulative distribution of frequencies (CDF) of both the experiment and simulations. This shows once again that the grain diameters of the experiments lie within the range of the simulated grain diameters.

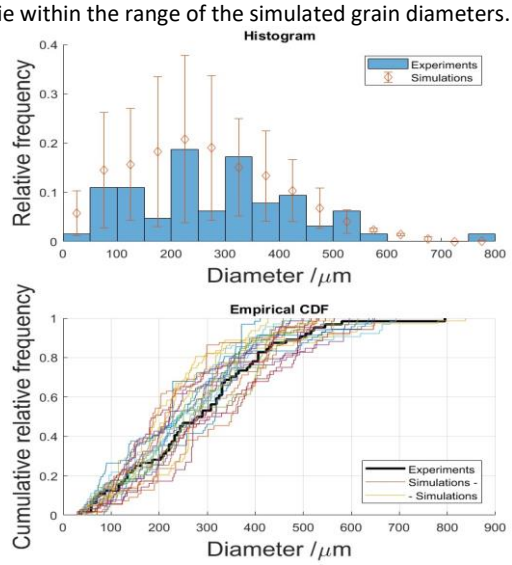

Figure 3. Histogram of the line diameters (top) and the cumulative distribution of frequencies for the experiments and the simulations. The mean value for the experiments is 284 µm with a standard deviation of 154 µm. For the simulations, the mean is 262 µm and the standard deviation is 137 µm.

5. Conclusion

In this paper, a CA is used to model the microstructural evolution in Ti-6Al-4V parts, produced by SLM during heat treatment. The micrographs of the initial microstructure are first analysed by using an automated image analysis script, and serve as input data for the CA. A comparison between the simulation and the experimental results after heat treatment show that the shape of the grains and the size distribution of the grains is similar, leading to the promising conclusion that a simple cellular automata is able to predict the proposed heat treatment. Future work will include the effect of crystallography on the growth speed, thus allowing to take into account directionality during heating. Furthermore, research will be performed to relate the microstructure to the mechanical properties in order to predict the effect of the morphology change.

Acknowledgements

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