PROCEEDINGS OF THE 9TH INTERNATIONAL SYMPOSIUM ON



ENERGY, AEROSPACE, AND INDUSTRIAL APPLICATIONS

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The Minerals, Metals & Materials Series

Eric Ott · Xingbo Liu · Joel Andersson Zhongnan Bi · Kevin Bockenstedt Ian Dempster · Jon Groh Karl Heck · Paul Jablonski Max Kaplan · Daisuke Nagahama Chantal Sudbrack Editors

Proceedings of the 9th International Symposium on Superalloy 718 & Derivatives: Energy, Aerospace, and Industrial Applications





Editors

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 ISSN 2367-1181
 ISSN 2367-1696 (electronic)

 The Minerals, Metals & Materials Series
 ISBN 978-3-319-89479-9
 ISBN 978-3-319-89480-5 (eBook)

 https://doi.org/10.1007/978-3-319-89480-5
 ISBN 978-3-319-89480-5
 ISBN 978-3-319-89480-5

Library of Congress Control Number: 2018937690

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Printed on acid-free paper

This Springer imprint is published by the registered company Springer International Publishing AG part of Springer Nature

The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

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Preface

This conference marks the 9th International Symposium on Superalloy 718 and Derivatives. The legacy which started in 1989 in Pittsburgh, Pennsylvania, continues to provide a rich forum for a combination of industrial and academic technical papers, presentations, and posters on highly relevant, high-temperature, superalloy materials. The strength of this series is in its breadth of technical, geographic, demographic, and application coverage. Over the years, it has provided an event for all those interested in high-temperature materials and reaches well beyond the simple exchange of technical findings. It is regularly a reunion for the many who work together solving development and production challenges at a distance from one another through ever-increasing electronic-enabled collaborations.

This 2018 proceedings volume consists of 72 papers; topic coverage includes the traditional subjects of casting, forging, and mechanical properties as well as topics on microstructure, joining, and novel processing. In the most recent two conferences, the advent of novel processing technologies including additive manufacturing has begun to open new avenues of investigation in what is a very dynamic field of engineering and science. Across the range of technology areas, the use of advanced characterization and modeling continues to make significant advances in the field. Contributions in this year's conference have spanned a wide swath of the industrialized world from Canada to South Korea and from the USA to Japan; 60% of papers come from outside the USA. Authors represent academic institutions (44%), laboratories (17%), and companies (36%). Although from a great diversity of areas and backgrounds, many gather to discuss knowns and unknowns and to forge ahead with enriching the understanding of metallurgy and application of these materials.

Our volunteer team has worked to bring a high quality and broadly relevant conference to authors and conference participants. We hope that the conference and these proceedings continue to enrich the advancement of understanding and application of these materials now and in the years to come.

> Eric Ott, Lead Editor Xingbo Liu, Organizer

Quantitative Texture Prediction of Epitaxial Columnar Grains in Alloy 718 Processed by Additive Manufacturing



Jian Liu, Qian Chen, Yunhao Zhao, Wei Xiong and Albert To

Abstract The lack of a reliable theoretical model of the processing-microstructure relationship of AM (Additive Manufacturing) material is preventing AM technology from being widely adopted by the manufacturing community. The goal of this work is to establish the link between the microstructure (texture) and the process parameters of metal AM processes. A quantitative method based on the epitaxial growth of columnar grains within and across melt pools is proposed to predict the texture formation during а metal AM process. The state-of-the-art CALPHAD-informed FEM (finite element method) simulation has been used to predict the geometry and thermal profile of the quasi-steady melt pool. The thermal gradient distribution within the 3D melt pool determines the crystallography direction and growth direction of the columnar grains within each deposited single tracks. The single tracks with the predicted geometry are amalgamated together to represent the bulk part, and the epitaxial growth of grains across the boundary of neighboring tracks are quantitatively modeled. The proposed method is calibrated and validated by experimental studies of metal AM processed Alloy 718.

Keywords Additive manufacturing • Inconel 718 • Microstructure

Introduction

The objective of this research is to develop a part-scale process-microstructure simulation tool to predict the microstructure evolution of Alloy 718 processed by powder bed laser fusion process integrating FEM thermal analysis and grain texture modeling. A great research interest of additive manufactured Alloy 718 is improving the performance of structural components for high temperature applications such as jet engine parts, where both creep and strength are critical and need to be designed for. The methodology developed in the proposed research will

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E. Ott et al. (Eds.), *Proceedings of the 9th International Symposium on Superalloy* 718 & Derivatives: Energy, Aerospace, and Industrial Applications, The Minerals, Metals & Materials Series, https://doi.org/10.1007/978-3-319-89480-5_49

introduce an efficient way to govern the in-situ microstructure evolution during laser process, which will directly drive the optimization for better mechanical properties of AM parts.

Modelling

FEM Thermal Modeling and Simulation of Single Track Depositions

The quasi-steady state melt pool profile within a single track is simulated by finite element thermal simulation using ANSYS FE software (Fig. 1a). The process parameters of P = 200 W and V = 1 m/s are employed in the case study in this report. The predicted thermal gradients versus solidification rates along the melt pool boundary in the X-Z plane are plotted against the columnar-to-equiaxed transition curves of Alloy 718 [1, 2] (Fig. 1b). From the FEM predicted G-R curves, it can be expected that the solidification is in columnar dendrite mode where our columnar grain growth model is applicable. The columnar dendrite mode is also verified by electron backscatter diffraction (EBSD) measurements. The FEM mode parameters, such as the absorption factor of laser power and the enhanced



Fig. 1 a The FEM prediction of a single track deposition, **b** predicted thermal gradients G (y-axis) versus solidification rates R (x-axis) along the melt pool boundary in center X-Z plane, against the curves of solidification mode transition between columnar to mixed mode (blue line) and mixed to equiaxed mode (red line) [1], **c** the predicted and experimented melt pool shape in Y-Z plane, **d** the predicted 3D melt pool geometry

conductivity factor within melt pool, were calibrated by correlating the predicted melt pool shape in the Y-Z plane with experimental result (Fig. 1c). The predicted 3D melt pool geometry (Fig. 1d) using the calibrated FEM model parameters are used as input for the grain growth model.

Columnar Grain Growth Model for Texture Prediction

A new Lagrangian approach for simulating columnar grain growth is proposed based on solidification theory. The solidification morphology of metals depending on the thermal gradient and solidification rate values at the solid-liquid interface [3]. In the case of columnar dendrite mode solidification in AM, dendrite arms will grow epitaxially from the seed crystal provided by the base metal, since the solid (base) metal and the liquid metal have similar chemical composition and the same crystal structure. Each dendrite arm will have the same crystallographic orientation as its seed crystal. The polycrystal base provides different seed crystals of different orientations at different locations. Within a small element surface around a point, the crystallographic orientation of the dendrite arm grow from this location can be determined if we know the 3D microstructure of the substrate. The growing direction of the dendrite will be along one of the <001> axis of its crystallographic orientation (the one that is most closely aligned with the local thermal gradient vector) [4]. In the proposed grain growth model, the dendrite arms were simplified as line segments and the growth of the arms will be simplified as the tracking of moving front point of each dendrite arm line. Such a Lagrangian approach is expected to be much more computationally efficient than the Eulerian approach such as cellular automaton [5-8]. At each step in the proposed approach, the growth direction of each dendrite arm line needs to be evaluated, since the local thermal gradient is changing, and hence the growth direction could change from one crystal <001> axis direction to another. While the dendrite arms grow from the same seed crystal are mostly parallel to each other, dendrite arms from different neighboring seed crystals will be either converging or diverging. For the converging case, the competition of dendrites and the growth of more preferred dendrites over the less preferred arms need to be incorporated into the model. For the diverging case, the branching mechanism needs to be incorporated to generate new dendrite arms to fill the gap between diverging primary dendrites. A 2D case demonstration of the grain growth model is shown in Fig. 2. After the growth, the dendrite arms grown from the same seed crystal will have identical crystallographic orientation and can be grouped into one columnar grain that has a 3D shape and volume. The resulting overall texture of one scan track can be obtained by adding each columnar grain orientation and its associated weight (volume) into a collection. An ideal shallow melt pool (W/D = 3) is employed as input to predict the grain growth and the resulting texture of a single track scan (Fig. 3). The computation time for such as a simulation was about 10 min on the desktop computer.

Fig. 2 The 2D case demonstration of the grain growth model: \mathbf{a} initializing the dendrites arms from seed crystals, \mathbf{b} dendrite lines during the growth simulation, \mathbf{c} finalized dendrite lines after growth simulation

Fig. 3 Predicted **a** columnar grain and **b** texture pattern of a single track with a shallow melt pool geometry

Validation of Grain Growth Model with EBSD Results

The columnar grain growth model is used to simulate 3D solidified grains within a single track. The ideal experimental validation would be a comparison with 3D EBSD measurement of the solidified grains utilizing FIB-SEM system. However, the experimental studies of the solidified grains are usually limited to EBSD measurement of 2D cross-sections (along Y-Z, X-Y, X-Z planes) of the printed track. Here we use EBSD measurement of the transverse (Y-Z plane) cross-section to validate the grain growth model (Fig. 4a). A single track of Alloy 718 was printed on a 1 mm thick substrate plate of the same material using the EOSINT DMLS M290 system. A cubic sample was cut from the plate around the deposited single track with one face perpendicular the track. This sample surface was prepared for EBSD. The EBSD measurement was used to construct the solidified grains within the transverse cross-section. The transverse cross-section

was also imaged under the optical microscope (OM) after etching to reveal the grain boundary (Fig. 4b). From the EBSD and OM results, the relevant grains are those that lie within the melt pool and across the melt pool boundary (Fig. 4c). The un-melted part of the grains (Fig. 4c) will serve as input to the grain growth model to predict the grain growth within melt pool. Since the experimental results are 2D, a thickness needs to be assumed to extend the 2D partially melted grains to 3D grains (Fig. 4d), which are then inserted into the virtually generated substrate microstructure (Fig. 4e). After the simulation of grain growth (Fig. 4f), the 2D cross-section of the simulated grains can be compared with experimental results.

Figure 5 is the transverse grain structure comparison of the experimental solidified grains based on EBSD measurement with the simulated grain by the columnar grain growth model. The process parameters are P = 200 W and V = 1 m/s. The input for the grain growth model was the FEM predicted melt pool geometry profile using the same process parameters and calibrated FEM model parameters. A good match between experimental and prediction can been observed in terms of the grain shape and orientation.

Fig. 4 The demonstration of the validating procedure for grain growth model using experimental measurement of the transverse cross-section: **a** EBSD measurement of the transverse cross-section of the single track, **b** the optical microscope image of the same cross-section, **c** the relevant grains that lie within the melt pool and across the melt pool boundary, **d** the un-melted part of the relevant grains that were extended from 2D cross-section measurement to 3D grains, **e** the virtually generated substrate microstructure at the begin of solidification with the inserted grains obtained by EBSD and **f** the microstructure after the simulation of grain growth

Fig. 5 Transverse grain structure of the single track of P = 200 W and V = 1 m/s: **a** the simulated grain by the columnar grain growth model and **b** the experimental solidified grains based on EBSD measurement

Conclusions

In this research, FEM thermal analysis of melt pool geometry and thermal profiles in single track depositions is performed and employed as input for texture prediction. An efficient epitaxial columnar grain growth model is developed to predict grain growth and resulting texture. EBSD measurement of the transverse (Y-Z plane) cross-section is then used to validate the grain growth model. A good match between prediction and experiments has been observed. The columnar grain growth model will be extended from single track to multiple tracks and multiple layers to study effects of processing parameters (hatching space, layer thickness and scanning strategy, etc.) on the texture evolution in 3D bulk part additive manufacturing.

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