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Microstructure-Property Correlations for the Design of New Materials

KIRUBEL TEFERRA

Multifunctional Materials Branch
Materials Science & Technology Division

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14. ABSTRACT

This document satisfies the closeout requirements for NRL base program 1J40: Microstructure-property correlations for the design of new materials. It provides an overview of the technical objectives of the program, technical progress, and dissemination of research findings through publications, reports, and presentations. The objective of the program is to develop a data analytics modeling framework to identify the effects of microstructural features on mechanical behavior relating to structural performance. A series of process-structure-property models were developed under this program within the Integrated Computational Materials Engineering framework, including microstructure solidification models, residual stress models for additively manufactured metals, and Gaussian process surrogate models, in order to predict the effect of additive manufactured build conditions on material mechanical behavior.

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CLOSEOUT MEMORANDUM FOR NRL BASE PROGRAM 1J40: MICROSTRUCTURE-PROPERTY CORRELATIONS FOR THE DESIGN OF NEW MATERIALS

1. PROGRAM DESCRIPTION

The objective of the program is to develop a data analytics modeling framework to identify the effects of microstructural features on mechanical behavior relating to structural performance. This program seeks to develop predictive models that relate stress and strain localization to the underlying microstructural features in order to improve the predictability of material failure. Improving the understanding of how material processing relates to microstructure formation and mechanical properties and performance will reduce the cost of novel materials development. In order to achieve program goals process-structure-property models were developed for additively manufactured metals. Process to microstructure modeling was developing using the cellular automata finite element (CAFE) model, which was modified to computationally efficiently model laser powder bed fusion processing. The CAFE code was interfaced with MOOSE Multiphysics Modeling Framework in order to conduct mechanical analysis of microstructural representative volume elements to predict material properties. One study was conducted that computed microstructural-resolved residual stress of as-built L-PBF 316L stainless steel, which demonstrated the role of polycrystalline heterogeneity on stress and strain localization. As these models are computationally expensive, Gaussian process surrogate models were developed that provide process-structure-property mappings by establishing functional relationships among the aforementioned computational models inputs and outputs. Below provides more details on the developed models and materials characterization to support model development. The publications and dissemination material produced under this program are listed at the end of this report, where more details of the studies can be found.

1.1 Microstructure Simulation

One thrust of the program has been to develop computational models to generate statistically equivalent virtual microstructures. These are digital microstructures that are generated such that they match the statistical features of a real material, which is collected through microstructural characterization. The first models developed under this program is a random tessellation model called Generalized Balanced Power Diagrams. This is a tessellation that generalizes the concept of a distance metric to control the region of a given grain. Training these models to material data often involves expensive optimization routines that are difficult to implement. Under this program, a simple, heuristic approach was developed that was shown to be just as good as costly optimization techniques while being able to determine model parameters in a trivial amount of time. This enabled fitting this type of tessellation model to practically-sized microstructures. However, while this model can represent traditional material microstructures that have grain morphologies that are nearly equiaxed, it cannot capture the complex microstructural features of additively manufactured (AM) materials.

Therefore, in order to properly model the microstructural solidification process and as-built microstructure for additive manufacturing, an in-house code of the cellular automata finite element (CAFE) model was

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developed. This model takes AM build conditions as input and outputs solidified, as-built microstructures. It does this by simulating the thermal field history during solidification and uses an empirically derived ther-

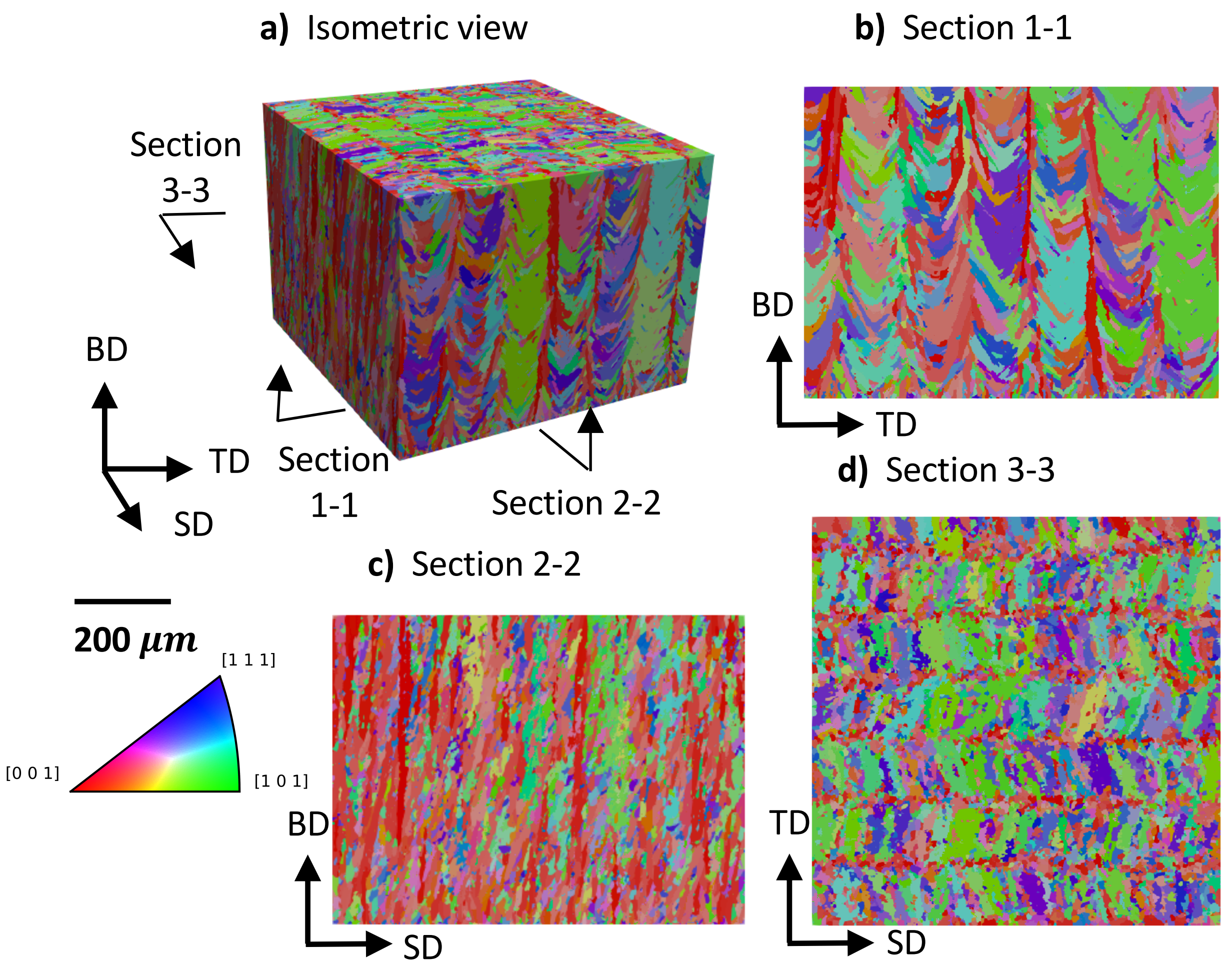

Fig. 1—Isometric view along with example SD, TD, and BD cross sections of L-PBF 316L built using a back and forth scan pattern.

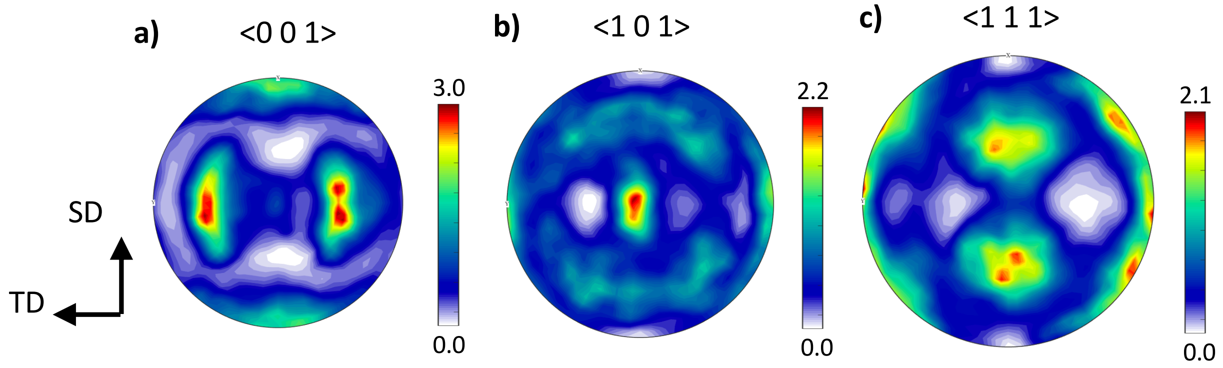

Fig. 2—Pole figures of the ⟨001⟩, ⟨101⟩, and ⟨111⟩ crystallographic directions for the simulation in Fig. 1.

1.2 Micromechanical modeling

A number of computational micromechanical models have been developed under this program. A computational homogenization technique was developed that performs Monte Carlo simulation of crystal plasticity finite element (CPFE) simulations of statistically equivalent microstructures. As these models are computationally expensive, the developed technique utilizes random field theory to represent the distribution of the homogenized properties to enable extrapolating the predicted properties for large domains based on simulations of smaller domains. In addition to homogenized properties, an analytical formula for the maximum value distribution of a random field was utilized to characterize micromechanical response quantities. In particular, the distribution of fatigue indicator parameters was quantified through this analytical model such that its distribution can be extrapolated for much larger domain sizes than simulated.

The CAFE model which simulates the solidified, as-built microstructure was coupled to thermomechanical finite element solver in the MOOSE Multiphysics Modeling Framework to predict the residual stress in the microstructure due to the thermal history during solidification. This model uses the crystal plasticity constitutive model to describe material behavior and is capable of capturing stress and strain distribution and concentration due to microstructural heterogeneity. This model enables relating residual stress and strain to input build conditions at the microscale. It was shown in this work that treating the material as homogeneous (i.e., not including polycrystalline morphology and crystallography) can tremendously underestimate the plasticity in the as-built material. Example simulation results showing the von Mises residual stress for 3 different build conditions along with analogous simulation using isotropic and homogeneous material properties are shown in Fig. 3.

This program also partially supported the PhD dissertation of colleague Dr. Robert Saunders. Under this program, a process-structure-property surrogate mapping was developed that links input build parameters to microstructure statistics, and microstructural statistics to material stress-strain curves. This approach constructs a database of CAFE simulations and mechanical responses using CPFE simulations. Then Gaussian process (GP) surrogate models are trained on this database to establish the aforementioned relationships. It was shown that the trained GP model was capable of accurately predicting the microstructural statistics and stress-strain curve for a build condition not included in its training. This suggests that the upfront effort of establishing the database is offset by the fast prediction of process-structure-property relations of the GP in order to explore the build parameter design space.

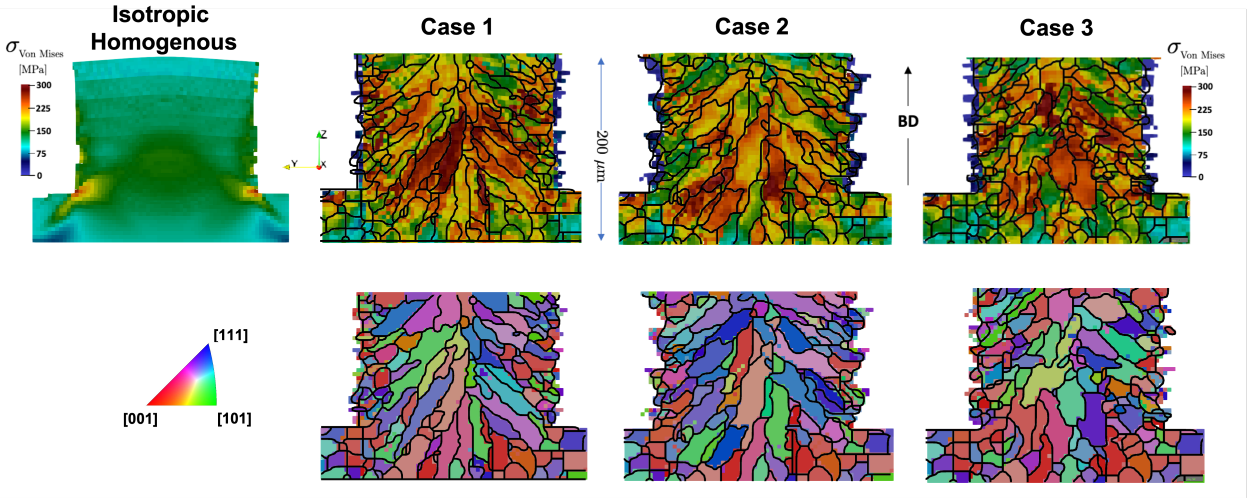

Fig. 3—Scan direction cross section cuts of the isotropic homogeneous and three cases examined mapped by average residual von Mises stress (top row) and grain orientation (bottom row).

1.3 Materials characterization

In conjunction with other programs, 3D characterization of AM microstructures has been conducted to collect and statistically analysis material data. In particular, detailed statistical processing of the tortuous grain morphology of large grains as well as the pore structure of an L-PBF 316L sample was conducted. The complex grain morphology of AM microstructures renders classical statistical representations such as grain size insignificant. Therefore, effort has been made to develop novel representative feature definitions as well as their statistical characterization. This includes using a watershed algorithm to decompose a grain into subdomain regions that can be fit to ellipsoids. It was found that the ellipsoidal primary axes align with one of the family of 6 $\langle 001 \rangle$ crystallographic directions, whose directions are strongly determined by the laser scan pattern. These results provide experimental verification that solidification is dominated by competitive epitaxial dendritic growth with strong $\langle 001 \rangle$ anisotropy, which is oriented along the melt pool boundary normal direction. This is a key finding for validating the presumptions of the CAFE model. Characterization efforts have been extended to mechanical properties, where samples were tested using high energy synchrotron X-rays enabling 3D characterization of strain distribution. These results are vital for validating crystal plasticity finite element models.

2. DISSEMINATION

2.1 Peer reviewed journal publications

1. Teferra, Kirubel, and Lori Graham-Brady. ”A random field-based method to estimate convergence of apparent properties in computational homogenization.” Computer Methods in Applied Mechanics and Engineering 330 (2018): 253-270. doi: https://doi.org/10.1016/j.cma.2017.10.027
2. Teferra, Kirubel, and David J. Rowenhorst. ”Direct parameter estimation for generalised balanced power diagrams.” Philosophical Magazine Letters 98.2 (2018): 79-87. doi: https://doi.org/10.1080/09500839.2018.1472399

3. Rowenhorst, J., Lily Nguyen, and Richard W. Fonda. ”3D Analysis of Large Volumes Through Automated Serial Sectioning David.” Microscopy and Microanalysis 24.S1 (2018): 552-553. doi: https://doi.org/10.1017/S1431927618003252
4. Teferra, Kirubel, and Lori Graham-Brady. ”Maximum Value Distribution of Micromechanical Response Quantities.” Journal of Engineering Mechanics 145.5 (2019): 06019002. doi: https://doi.org/10.1061/(ASCE)EM.1943-7889.0001612
5. Brewick, Patrick T., Stuart I. Wright, and David J. Rowenhorst. ”NLPAR: Non-local smoothing for enhanced EBSD pattern indexing.” Ultramicroscopy 200 (2019): 50-61. doi: https://doi.org/10.1016/j.ultramic.2019.02.013
6. Murphy-Leonard, Aeriel D., et al. ”Investigation of porosity, texture, and deformation behavior using high energy X-rays during in-situ tensile loading in additively manufactured 316L stainless steel.” Materials Science and Engineering: A 810 (2021): 141034. doi: https://doi.org/10.1016/j.msea.2021.141034
7. Teferra, Kirubel, and David J. Rowenhorst. ”Optimizing the cellular automata finite element model for additive manufacturing to simulate large microstructures.” Acta Materialia 213 (2021): 116930. doi: https://doi.org/10.1016/j.actamat.2021.116930
8. Saunders, Robert N., Kirubel Teferra, Alaa Elwany, John G. Michopoulos, Dimitris Lagoudas, ”Metal AM Process-Structure-Property Relational Linkages using Gaussian Process Surrogates”, Additive Manufacturing (2023):103398. doi: https://doi.org/10.1016/j.addma.2023.103398
9. Yaghoobi , Mohammadreza, Krzysztof S Stopka, David L McDowell, Lori Graham-Brady, and Kirubel Teferra, ”Effect of sample size on the maximum value distribution of fatigue driving forces in metals and alloys”, Journal of the Mechanics and Physics of Solids (under review)
10. Kuna, Lukasz, and Kirubel Teferra. ”A Framework for Predicting As-Built Additively Manufactured Microstructures and Residual Mechanical Properties.” (manuscript in preparation)

2.2 Invited presentations

1. Teferra, Kirubel, ”Optimizing the cellular automata finite element model for additive manufacturing to simulate large microstructures,” Lawrence Livermore National Laboratory, (delivered virtually) November 24 2020
2. Rowenhorst, David J. U.S. Nuclear Regulatory Commission’s (NRC’s) Workshop on Advanced Manufacturing Technologies for Nuclear Applications: ”Linking 3D Microstructural Analysis of Additive Manufactured 316L to Performance and Properties in LPBF 316L”. December 7, 2020
3. Kuna, Lukasz, and Kirubel Teferra, ”Predicting as-built additively manufactured microstructures and residual stress using the CAFE model,” In the 6th World Congress on Integrated Computational Materials Engineering April 25, 2022 (invited session keynote)
4. Teferra, Kirubel, ”Microstructure solidification and residual stress modeling of metal additive manufacturing,” University of Texas at San Antonio Department of Mechanical Engineering Seminar, September 16, 2022
5. Teferra, Kirubel, ”Computational modeling of solidification, residual stress, and uncertainty quantification in metal additive manufacturing,” University of Arizona Department of Aerospace and Mechanical Engineering Seminar, October 27, 2022

2.3 Released software

1. AMCAFE: https://github.com/USNavalResearchLaboratory/AMCAFE

2.4 Conference presentations

1. Kirubel Teferra, Lily Nguyen, and David J. Rowenhorst. Generating statistically equivalent synthetic microstructures of additively manufactured stainless steel. In the 13th World Congress on Computational Mechanics WCCM, New York, NY, July 23?27 2018
2. Kirubel Teferra and David J. Rowenhorst. Towards simulating microstructure evolution of 3D printed stainless steel using the cellular automata finite element model. In the 15th US National Congress on Computational Mechanics USNCCM, Austin, TX, July 28-August 1 2019;
3. Kirubel Teferra and David J. Rowenhorst. Optimizing the cellular automata finite element model for additive manufacturing to simulate large microstructures. In the 14th World Congress on Computational Mechanics (WCCM), virtual, January 11-15 2021
4. Kirubel Teferra and David J. Rowenhorst. Optimizing and validating the cellular automata finite element model for additive manufacturing. The 150th Annual Meeting of the Minerals, Metals, and Materials Society (TMS) (TMS 2021) (delivered virtually), March 14-18, 2021
5. David J. Rowenhorst. 3D Analysis of Grain Morphologies and Solidification Texture in AM 316L. The 150th Annual Meeting of the Minerals, Metals, and Materials Society (TMS) (TMS 2021) (delivered virtually), March 14-18, 2021
6. David J. Rowenhorst. Analysis of Grain Structures and Voids within Additive Manufactured 316L by Serial Sectioning. 3D Materials Science 2021 (delivered virtually)
7. Lukasz Kuna and Kirubel Teferra. Utilizing the Cellular Automata Finite Element model to simulate thin wall microstructures of 3D printed metals. In the 16th U.S. National Congress on Computational Mechanics (USNCCM), (delivered virtually), July 25-29, 2021
8. Lukasz Kuna and Kirubel Teferra. Modeling microstructure solidification and residual stress of as-built additively manufactured materials. In the Engineering Mechanics Institute (EMI) Conference, May 31-June 3 2022
9. Marissa Linne, Jean-Baptiste Forien, Nicolas Bertin, Margaret Wu, Sylvie Aubry, Tatu Pinomaa, Anssi Laukkanen, Kirubel Teferra, Nathan Barton, Y. Morris Wang, and Thomas Voisin. Investigation of the microstructure and plastic deformation of am 316L stainless steels. In the 151th Minerals Metals & Materials Society Conference (TMS2021), virtual, March 15-18 2022
10. Jean-Baptiste Forien, Nicolas Bertin, Tatu Pinomaa, Anssi Laukkanen, Kirubel Teferra, Margaret Wu, Marissa Linne, Sylvie Aubry, Nathan Barton, Y. Morris Wang, and Thomas Voisin. Characterization of microstructures and deformation mechanisms in additively manufactured 316L stainless steels. In the 6th International Congress on 3D Materials Science (3DMS 2022), (invited session keynote), June 26-29 2022
11. Kirubel Teferra and Lukasz Kuna. Simulating the effect of processing conditions on microstructure-resolved residual stress. In the 1st DoD Basic Research Conference, Sept 6- 9 2022