PREDICTING MICROSTRUCTURE-SENSITIVE FRACTURE BEHAVIOR IN AM IN625 USING A DAMAGE-ENABLED ELASTO-VISCOPLASTIC FFT FRAMEWORK

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Abstract

In this work, we use a large-strain elasto-viscoplastic fast Fourier transform (LS-EVPFFT) code enhanced with a continuum damage mechanics model to predict failure response of a subcontinuum mesoscale tensile specimen in the context of the National Institute of Standards and Technology (NIST) 2022 Additive Manufacturing Benchmark (AM-Bench) Challenge. In the Challenge, participants were provided with data from X-ray computed tomography and electron backscattered diffraction (EBSD) for an AM IN625 sample and asked to predict stress and strain response and locations of necking and fracture. To account for uncertainty in the subsurface microstructure, we instantiated 10 semi-synthetic microstructures using a Potts model in a modified version of the open-source software SPPARKS. While all 10 models maintain identical surface grain structure, surface roughness, and internal porosity, their subsurface grain structures vary due to randomness in the microstructure-generation procedure. Results from the blind predictions using the LS-EVPFFT framework are compared to the experimental results. Lessons learned are discussed.

1. Introduction

Literature shows that microstructural features of additively manufactured materials can vary dramatically in comparison to those of conventionally manufactured materials. Such microstructural features include grain and sub-grain structures as well as pore or void defects. The degree to which each type of feature influences the mechanical behavior of additively manufactured materials depends upon the mechanical property of interest and the prominence of the features relative to one another. For example, certain mechanical properties, like fracture and fatigue, tend to be more sensitive than other properties, like elastic modulus and yield strength, to pore or void defects. At the same time, the relative influence of such defects might depend upon the amount of residual stress in a built part, which can manifest in the development of complex sub-grain structures. In terms of modeling the impact of such microstructural attributes on mechanical behavior of additively manufactured materials, modelers must strike a balance between representing the relevant microstructural features with sufficient fidelity to capture the physics or mechanics at hand and maintaining computational tractability.

The NIST AM-Bench is a formal modeling challenge series designed and released broadly to the international modeling community to test the ability of both models and modelers to predict various aspects of (process-)structure-property relationships in AM. In the 2022 NIST AM-Bench, a limited set of experimental data was provided to participants, who were then given 12 weeks to submit blind predictions of specific metrics of interest. In Challenge 4 of the 2022 NIST AM-Bench, participants were asked to predict the mechanical response and fracture location of a mesoscale tensile specimen of AM IN625 produced by laser powder bed fusion. The specimen had nominal cross-sectional dimensions of 200 × 200 μm and a gauge length of 2.0 mm. Data provided to participants included parameters of the build, a stack of grayscale images from high-resolution X-ray computed tomography, and a map of the grain structure on one surface of the gauge section from EBSD.

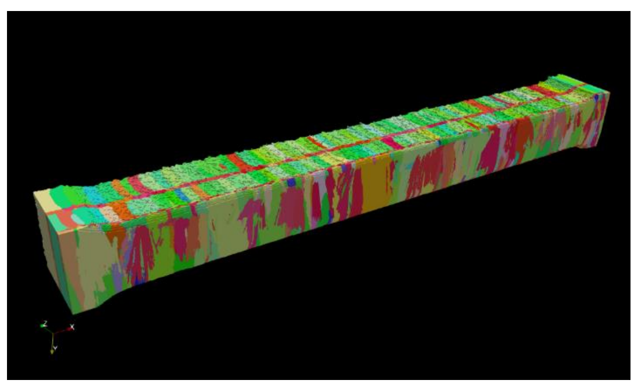

Figure 1 One of 10 microstructure instantiations generated for the 2022 NIST AM-Bench modeling challenge.

In this work, we describe our recent participation in Challenge 4 of the 2022 NIST AM-Bench using an LS-EVPFFT framework that was recently augmented to include a continuum damage mechanics model. The LS-EVPFFT framework includes a crystal plasticity constitutive model that accounts for plastic deformation through the evolution of crystallographic slip and a phenomenological hardening model. The continuum damage mechanics model assumes that fracture is driven by stress triaxiality. After identifying a target stress-strain response from the literature, the model parameters were calibrated. To account for uncertainty in the subsurface microstructure of the mesoscale tensile specimen, 10 semi-synthetic microstructure instantiations were generated. All instantiations had identical surface grain structure that conformed to the EBSD-generated grain map provided by NIST. However, the instantiations exhibited variable subsurface microstructure. An example instantiation is provided in Figure 1. Tensile loading to failure was then simulated for all 10 instantiations.

2. Results

Results from the 10 ductile fracture simulations were averaged to provide ensemble predictions of the stress-strain response. Table 1 provides the submitted values from the ensemble predictions. Among all predictions submitted by challenge participants, those listed in Table 1 achieved the lowest overall error, and the team was awarded First Place in the mechanical response predictions. Results from the simulations showed that the predicted fracture locations were sensitive to the subsurface microstructure, as illustrated in Figure 2. For the challenge submission, predicted fracture locations were averaged among seven out of the 10 simulations; three of the 10 predictions were considered outliers and discarded from the averaging.

Table 1. Submitted values from blind predictions compared to experimental values.

	Predicted (submitted) value	**Experimental value(s)**
Elastic modulus (GPa)	148	102
0.2% offset yield strength (MPa)	783	689
Ultimate tensile strength (MPa)	1098	1017-1073
True strain at UTS (mm/mm)	0.208	0.136-0.173
True stress at 0.05 true strain (MPa)	881	841

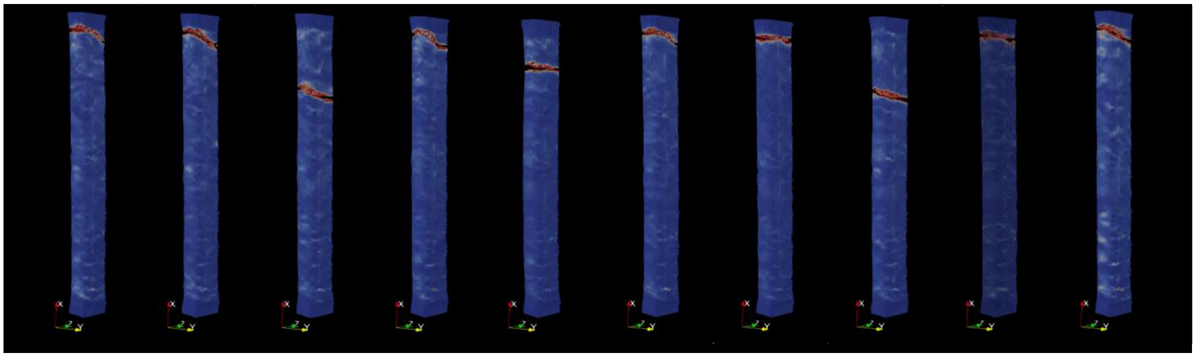

Figure 2 Predicted fracture locations for 10 microstructure instantiations.

3. Conclusions

Based on our results, we conclude that careful calibration of constitutive and damage/fracture parameters is critical to making accurate predictions of microstructure-sensitive failure response of AM materials. Subsurface microstructure is found to have a significant influence on location of fracture, and, unlike in many other cases, pore structure does not seem to have governed failure in the AM specimen studied here.

Acknowledgements

We gratefully acknowledge Drs. Ricardo Lebensohn and Miroslav Zecevic for their contributions to the implementation of the damage model that was used in this work. Computing resources were provided by the Center for High-Performance Computing (CHPC) at the University of Utah.