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Utilizing a Dynamic Segmentation Convolutional Neural Network for Microstructure Analysis of Additively Manufactured Superalloy 718

Stephen Taller, Luke Scime and Kurt Terrani

Oak Ridge National Laboratory, United States

Additive manufacturing (AM) is revolutionizing almost all industries through the production of intricate geometries that were previously prohibited by cost or machinability. Ni-based superalloys form a primary alloy class for high-temperature applications in the petrochemical, aerospace, and nuclear industries because of their intrinsic resistance to creep and high strength. Despite these attractive properties, the extreme work hardening of Ni-based superalloys [1] makes traditional manufacturing of complex shapes difficult, so these alloys are an attractive target for AM. Superalloy 718 was chosen as an example superalloy because of the wide variety of precipitates that can form within its composition space from the repetitive heating and cooling cycles of the AM process. The precipitates and other microstructure features will dictate the mechanical properties, so there is a significant challenge to characterize the size, number density, composition, and volume fraction of each microstructural feature from AM fabrication using analytical electron microscopy.

This work focused on the application of a pixel-wise classification machine learning (ML) model called a *dynamic segmentation convolutional neural network* (DSCNN) to identify the microstructural features of an as-fabricated additively manufactured superalloy 718. The specimen was produced using laser powder bed fusion on the Concept X-Line 2000R at the Manufacturing Demonstration Facility at Oak Ridge National Laboratory (ORNL), and it was examined using the FEI Talos F200X at the Low Activation Materials Development and Analysis laboratory at ORNL. Scanning transmission electron microscopy (STEM) was chosen over conventional TEM because it collects data across four detectors simultaneously for STEM bright field (BF), two annular dark field (DF1 and DF2), and high angle annular dark field (HAADF) images. In addition, the SuperX energy dispersive spectroscopy (EDS) system allows for x-ray spectra collection for each pixel, adding an elemental component to the dataset. Examples of the electron images and colorized EDS intensity maps from Kα x-rays for select elements are shown in Figure 1. In practice, the DSCNN works with any input imaging mode and can be used for almost any electron microscopy that results in an image.

The ML algorithm used is a DSCNN that was originally developed to detect defects during additive manufacturing at ORNL [2]. The DSCNN accepts an arbitrary number of input images of arbitrary resolution while ensuring that the output segmentation is always at the input image resolution. Three parallel legs encode information at multiple size scales, enabling the use of global and local information for segmentation. Deep morphological features are extracted with the U-net leg of the DSCNN while recalling approximate spatial locations. The low-resolution leg is a simple convolutional neural network which has a receptive field equal to the entire image. The high-resolution localization leg always has a receptive field which can be dynamically configured by the user, guaranteeing pixel-wise classification at the native input resolution. It also provides sublinear analysis times: that is, doubling the image resolution will not double the inference time. Together, these three legs form a model that can provide microstructural identification with near real-time identification.

Traditional CNNs are hindered by the requirement of hundreds of images with many individual features in which to train the network and by their high computational cost. The DSCNN, like other segmentation neural networks, uses pixel-wise information to reduce the necessary training set to a minimum of 100,000 pixels per class. Thus, the training of the DSCNN for superalloy 718 could be performed on a small image set with complementary EDS maps that includes representation of each microstructural feature. A simple pipeline was created in the Python environment to facilitate commonality (resolution, file format) among the STEM images and EDS x-ray spectra maps to feed into the DSCNN, as shown in Figure 2. Image labelling for the training dataset was performed within a custom user interface developed for this application. The DSCNN was trained with 24 input channels (4 STEM images, 10 EDS x-ray intensity maps, and 10 EDS quantified maps using the Cliff-Lorimer method [3]) to identify and classify 10 classes of features: the matrix γ phase, precipitating phases (γ′, γ″, δ, Laves, carbides), grain boundaries, dislocations, oxides, and platinum from the focused ion beam (FIB) lamella liftout process. Training and identification were performed on a commercially available desktop computer. A performance comparison with human experts to determine measures of precision and recall on a test dataset separate from the training dataset is still in development. Nevertheless, the implementation of a DSCNN on relatively low-cost, commonly available hardware will be beneficial to the microstructure analysis community.

The ultimate intent of this effort is to demonstrate a generalized approach for characterization of complex microstructures at large scale. This is being made possible through (1) advances in microscopy and its automation to assess large areas of the material (~ 2–3 orders of magnitude greater than what is usually performed) and (2) advances in pixel-wise machine learning classification tools that are agnostic to the image size, type, and number of input channels. This generalized approach will allow for an unprecedented view into materials microstructure that in turn facilitates more accurate prediction of their properties and rich source of data for design of new high-performance materials.

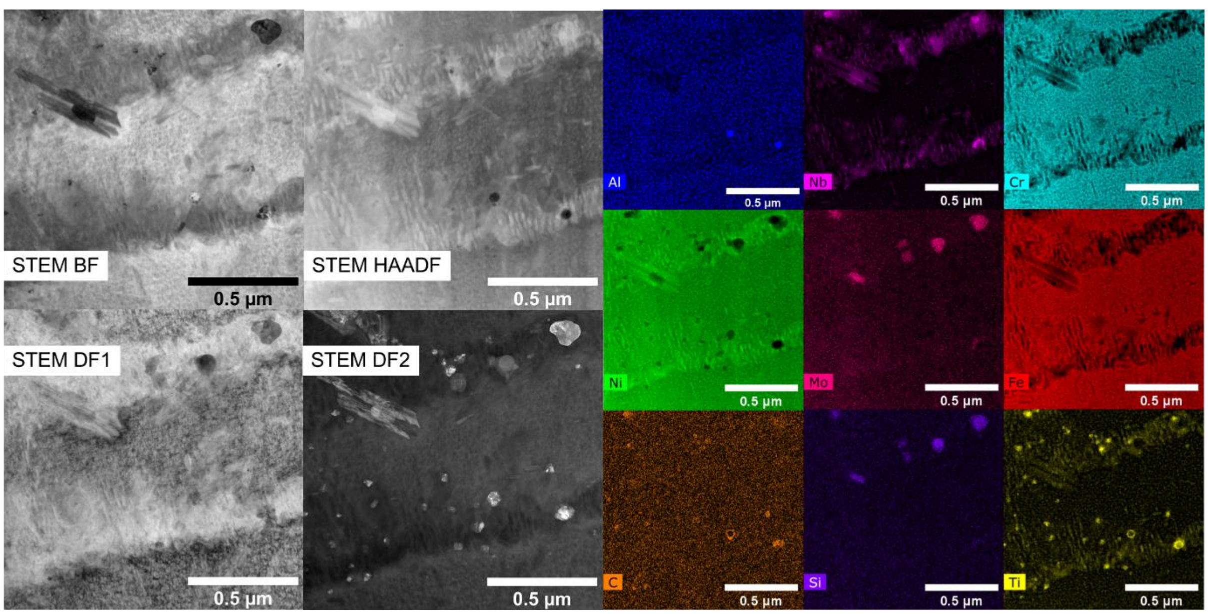

Figure 1. Figure 1. Examples of STEM images and EDS intensity maps from additively manufactured superalloy 718 for input into the DSCNN for feature identification with added labels.

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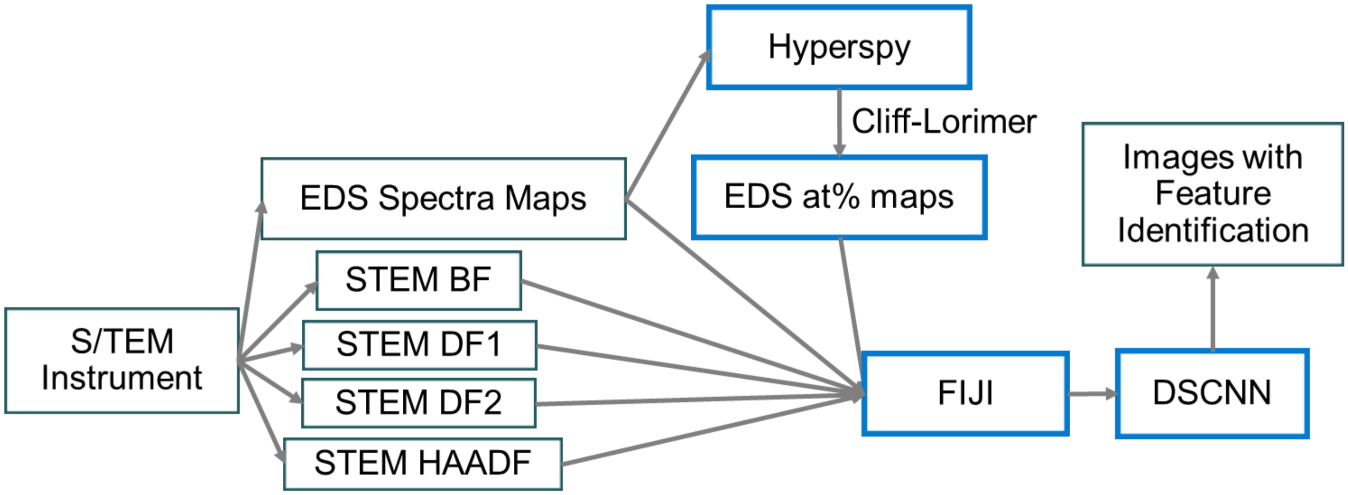

Figure 2. Figure 2. Flowchart from the acquisition of images on the S/TEM instrument through a series of custom Python scripts to analyze the images and EDS maps to identify precipitates and other microstructural features.

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