Characterization of Material Micro & Nano Structures Using Machine Learning Algorithms

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Abstract

In collaboration with Pacific Northwest National Laboratory, Embry-Riddle students are working on material classification of microstructural features obtained from scanning transmission electron microscopy (STEM) is attempted using various machine learning algorithms. STEM produces a micrograph of the material, which is fed through a segmentation and classification paradigm to identify the microstructures present. The initial research by the PNNL uses a few-shot method which allows the model to be operated using limited data. Using data from a sample micrograph, a new neural network is implemented with the objective of aptly segmenting the micrograph and obtaining classifications for the microstructures. This model investigates the use of existing image segmentation techniques, particularly region-based techniques. This approach is deemed appropriate since it is expected that the microstructures are grouped together by type. The success of this approach can provide a rapid and reconfigurable tool for identifying these microstructures.

Introduction

Material science is the study of how materials behave under various stresses and strains, as well as how the microstructures of these materials can affect their properties at the microscopic scale. It is essential to analyze changes to material properties at the atomic scale using the method of STEM to produce micrographs. From these micrographs, there are distinct variations of the pixels that represent a certain material from which needs to be identified and grouped for further classification. The goal of this project is to collaborate and design mathematical algorithms through deep learning to analyze the material subgroups from image classification. Specifically for this investigation, deep neural networks are trained to assign image data to different categories or classes as part of the task for material labeling and semantic segmentation.

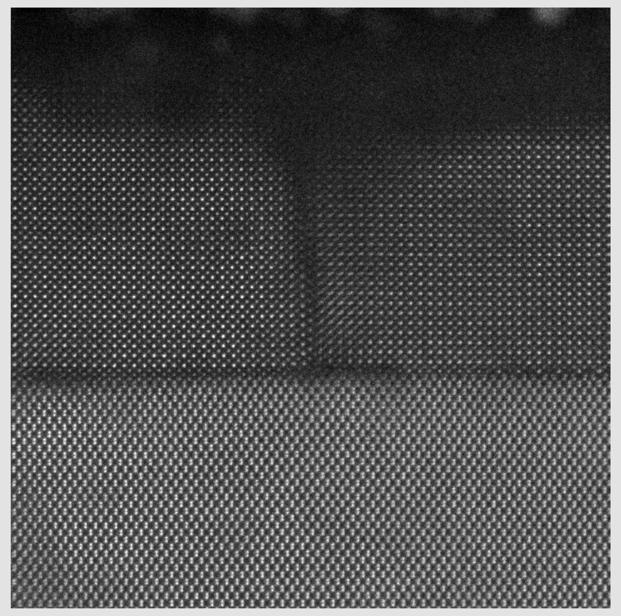


Figure 1: Sample STEM Micrograph of material containing STO, GE, and PT/C

Methodology

Semantic segmentation of the STEM micrograph is performed using a custom-built U-Net: a convolution neural network that consists of a contraction path and an expansion path.
The network model consists of 5 convolution layers in the contraction path and 4 convolutional layers in the expansion layers. Additionally, there exists 4 skip layers that allow for a future layer to have information from a preceding layer. This reduces the error induced by information abstraction. A final convolution layer is applied with a *1x1* kernel size and *n* filters, where n is the number of classes. In this final layer, a *softmax* activation function is used such that each material is classified as a unique class.

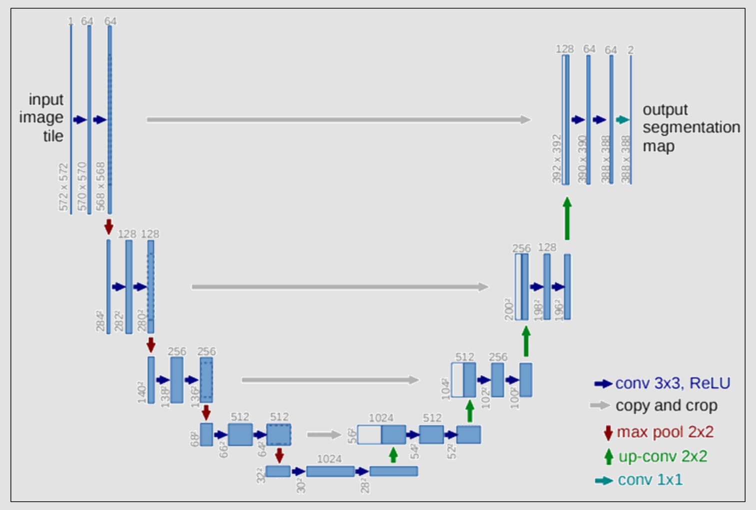


Figure 2: Proposed custom U-Net Architecture

A separate methodology involving the creation of custom alternating Convolutional Neural Networks (CNNs) and grid cleaning algorithms is currently in development. Training data consists exclusively of five labeled subsections, or "chips", from each of the three classes intended for segmentation.

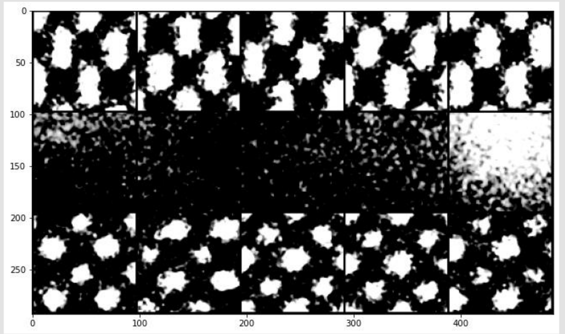


Figure 3: Transformed and normalized training data

The first CNN consists of two alternating layers of convolutional and max pooling layers, followed by three linear layers. The resulting model is applied individually to each non-training chip from the image, with one of three classes being assigned. The resulting image is tuned to segment one of the classes, stitched together, and then "cleaned" via cellular automaton algorithm biased towards extinction of small groupings of free-floating data.. This process is intended to be carried out a second time to segment the remaining two classes.

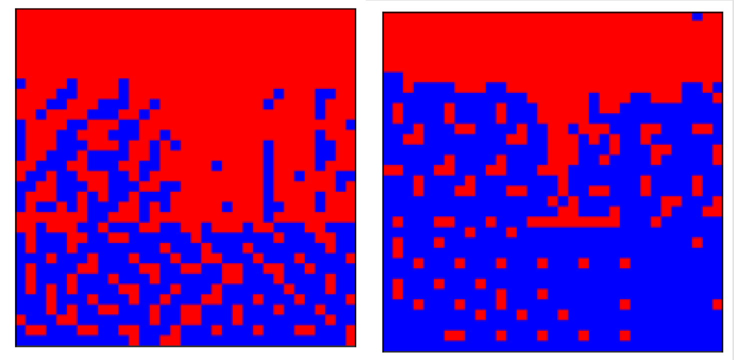


Figure 4: Pre-optimized (left) and Post-optimized (right) CNN output.

With the help of machine learning such as N-shot learning and Transferred Learning, it may provide new methods of automatically segmenting and analyzing pixels to determine what materials exist within a sample. Creating this new algorithm will help analyze, segment and cluster STEM micrographs' pixels at a more efficient rate. We want to combine Voronoi Diagrams, **Z**ero-**S**hot **L**earning (ZSL) with Transferred learning to allow the model to optimize performance time as it continues to cluster and classify for every unique STEM micrograph.

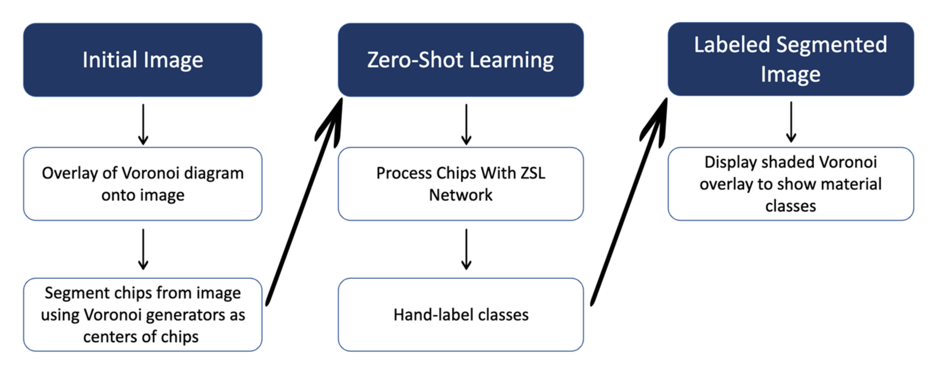


Figure 5. Initial Strategy & Process—The figure above displays the approach of automating the time consuming process by using Voronoi diagrams for feature segmentations and Zero-Shot Learning to cluster/classify features together to reduce the time needed for hand labeling of features on STEM micrographs

Results

The input image is a grayscale micrograph, which is processed through the deep learning model. Training at only 100 epochs and using a Categorical Cross Entropy loss function, the designed U-Net model is able to classify the materials as shown below.

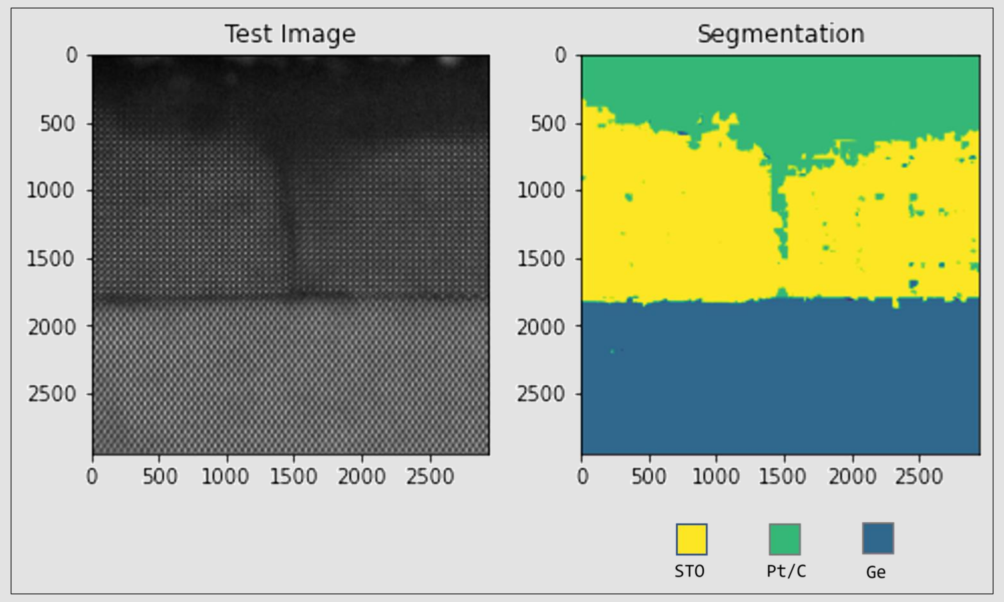


Figure 6: Results of Semantic Segmentation using U-Net model

The secondary method in development results in the segmentation shown in Figure 6. This method has a high success rate segmenting one of the classes using a single iteration of a CNN and grid cleaning algorithm.

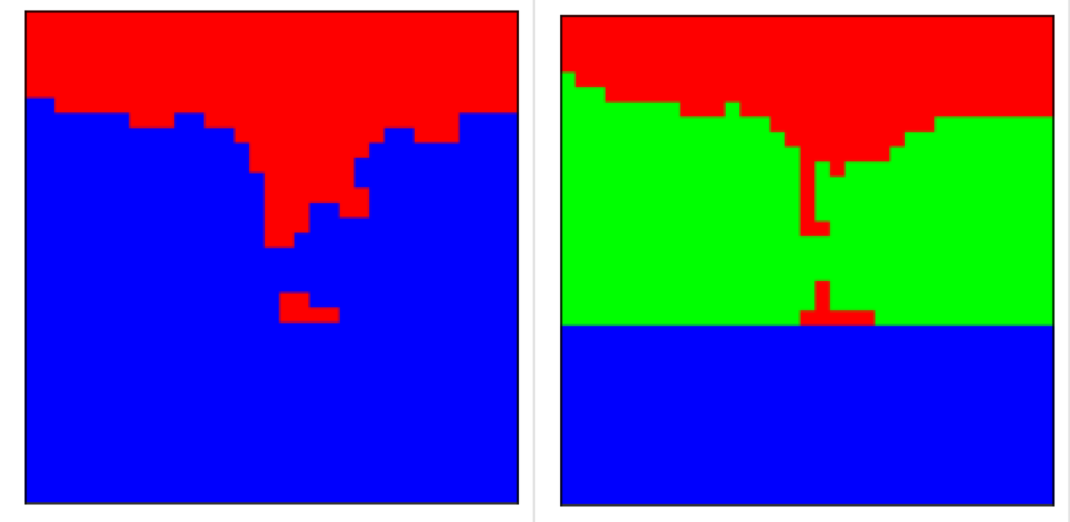


Figure 7: Post-1st Iteration Cleaning Algorithm (left) and Truth Data (Right)

A further iteration of a modified CNN and cleaning algorithm is intended to further segment the Germanium classified region (blue) in the left half of Figure 6 with the Strontium Titanium Oxide (green) region seen represented in the right half of Figure 6, which is the known truthful data.

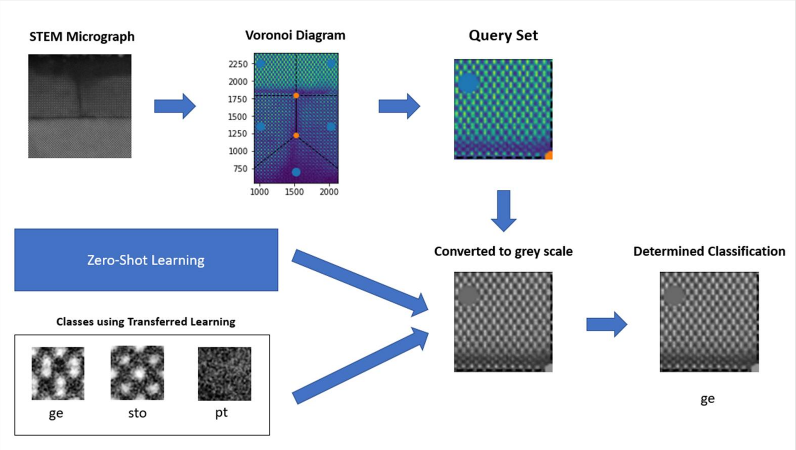
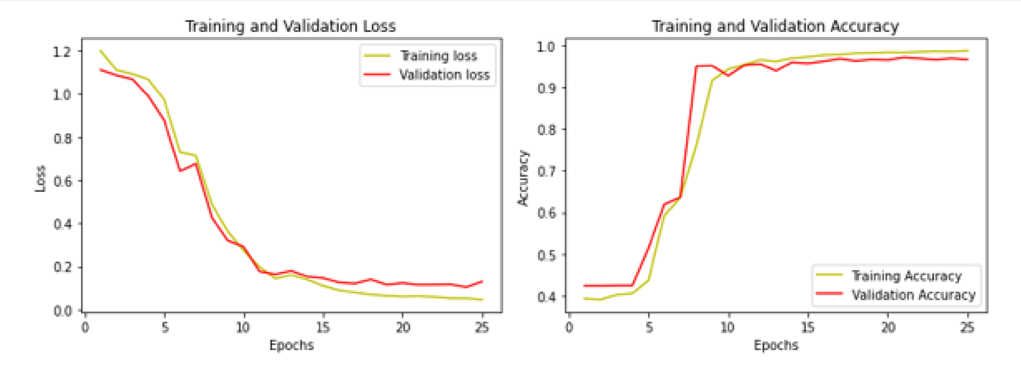


Figure 8. Zero-Shot Learning & Transferred Learning — The algorithm starts with the STEM micrograph, then overlays a Voronoi Diagram to begin segmenting similar features together. After the image is segmented, the query set is pipelined into the ZSL model and previous classifications using Transferred Learning will also the ZSL to determine the what materials the segmented image is comprised of.

Conclusion

- Jaccard Similarity Coefficient aka the Intersection Over Union statistic yielded a 96.5516% accuracy rate.
- Using Categorical Cross Entropy, the values for training and validation demonstrates consistent rates for both loss and accuracy.
- Final output showcases small amounts of error in segmentation as there is small evidence of mislabeling primarily in regards to the Germanium (Ge) subgroup.
- CNNs working in combination with other algorithms show promise towards segmentation of images with little training data available.



Recommendations

- To promote training efficiency, therein lies the possibility of generating artificial data as an addition to the support set provided using data augmentation techniques.
- The use of transfer learning and implementing a pre-trained model such as ResNet or VGG19 for the purpose of training existing networks with minimal data.
- Implementation of Generative Adversarial Network (GAN) which is an unsupervised neural network in machine learning where two separate networks compete for higher levels of accuracy in prediction processes of image classification and segmentation.
- Identifying potential relationships between chip size and known features could lead to development of cleaning algorithms with increased accuracy.

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