Research Proposal for MSA Undergraduate Research Scholarship

Undergraduate Researcher: Nidhish Sagar

Research Advisor: Will Bowman, Assistant Prof., Materials Science & Engineering, UC Irvine

Title

Algorithm for detection and tracking of grain boundaries in scanning transmission electron microscopy (STEM) videos of polycrystalline materials

Introduction

An electron microscope (EM) is an integral tool for a materials scientist. The EM of present day depends heavily on the presence of a trained user for viewing and characterizing desired micro/nanostructures. Even with well-trained and experienced users, however, collecting a statistically significant quantity of experimental data can be a challenging bottleneck to overcome for the microscopist. For example, characterizing grain boundaries in polycrystalline materials is a time-consuming task which is critical to understand many materials properties and behaviors. **The main goal of this proposal is to establish a robust and flexible video processing algorithm capable of rapid detection and tracking of grain boundaries in polycrystalline materials in annular dark field STEM videos.**

The Bowman Lab has been developing a novel machine vision-enabled automated STEM imaging and spectroscopic data acquisition system optimized for detection, tracking and nano characterization of grain boundaries in polycrystalline materials (Figure 1). Grain boundary tracking algorithms will guide targeted spectroscopic (e.g. electron energy-loss spectroscopy (EELS)) data acquisition needed to characterize static and dynamic composition and the electronic structure. A video showing a basic tracking algorithm for nanoparticle diameter and location during coalescence can be found online [3]. The Bowman Lab has also successfully demonstrated programmatic control over the STEM EELS data acquisition via a software platform developed in the Lab. The major challenge facing further implementation in experiments is optimizing the 'intelligence' of the software with respect to its ability to locate and track grain boundaries in STEM images.

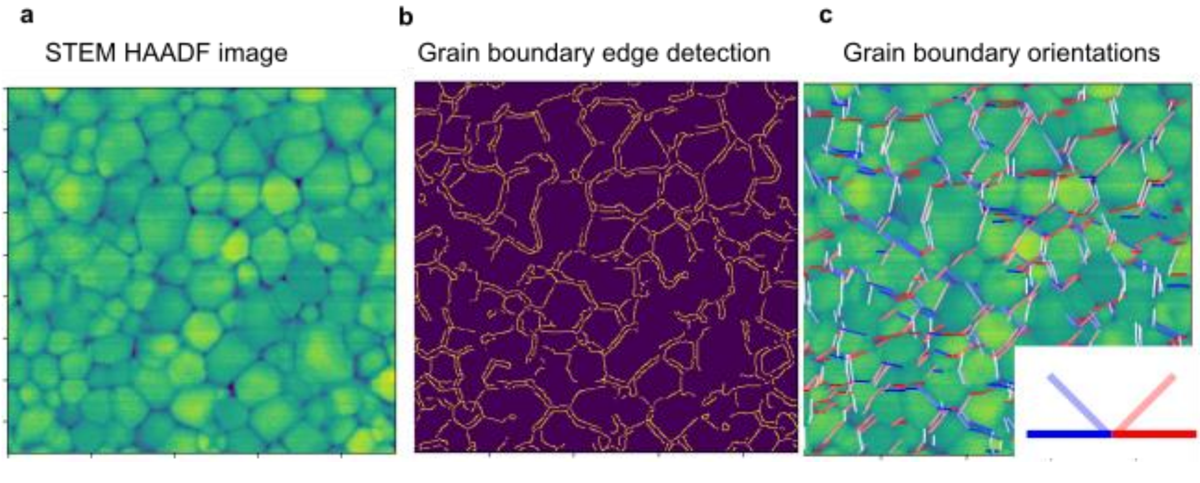

Figure 1. We are developing machine vision algorithms to optimize grain boundary (GB) detection and tracking. For example, GBs in a STEM annular dark field image of a polycrystalline fluorite oxide

(a) can be detected using robust edge-finding algorithms (b) and their spatial orientation can be determined automatically (c). We are in the process of integrating this software in an integrated STEM spectroscopic data acquisition system for high-throughput GB characterization.

Grain boundaries (GB) are of interest to the Bowman Lab because GB network composition and grain size determine the overall ionic conductivity of key materials used in energy storage and conversion applications, which in turn varies throughout processing of the polycrystalline microstructure. The chemical composition of GBs (i.e. point defect concentration) is directly correlated with the ionic diffusion across GBs and through the entire material [1,2], so understanding how the GB composition varies during processing is crucial for process design. This hypothesis can be tested using the algorithms developed in this study. The composition distribution of GBs is thought to be related to the crystallographic orientation of the crystalline grains in solid oxide electrolytes.

Methods

Systems for nanoparticle tracking and analysis by TEM have recently been reported, though specific domain knowledge will be needed to develop a system able to accurately and reliably detect, track and analyze GBs algorithmically[4].

Constructing computational Neural Networks can train the microscope to detect features of the sample and its surface. The task would involve in-depth understanding of Microscope hardware which is vendor based. Knowing the hardware will allow control of different components through Python programming. Using data from multiple EM images, we will train the computer to understand our requirements and specifications. The code will be run on the computer controlling the microscope and we expect the microscope to automatically focus the electron beam to obtain optimum resolution and detect surface features in an intelligent and quick way.

Description of Study's Goals

This work will establish a robust video processing algorithm for rapid detection and tracking of grain boundaries in annular dark field STEM videos.

This algorithm is a critical component of a larger microscope-control software platform that is being developed by the Bowman Lab. A major outcome of this project will be the demonstration of GB tracking on real-time STEM videos. The algorithm will be optimized for various STEM image magnifications, which can be challenging because the image/video pixel size relative to the object of interest can vary drastically as magnification is changed; however, this is important because magnification changes are practically critical to successful experiments. The algorithm will also handle changes in STEM video frame rate, where fast frame acquisition results in noisier images with lower signal to noise and vice versa for slow frame acquisition. The drawback of slow frame rates are that specimen motion and dynamic changes in the loci of grain boundaries may not be captured accurately. There are two approaches currently being explored in the lab for rapid and accurate GB detection and tracking: (1) Conventional edge-detection and (2) a machine learning approach to image object detection.

Future work on the software platform will focus on processing the large datasets comprising multidimensional spectral data acquired from various locations in the STEM specimen and at various times during the STEM experiment. Challenges will likely arise from interpreting the chemical information in the spectral data and correlating that back to the STEM specimen in a statistically reliable and physically meaningful way.

Through this study, our aim is to reduce the effort of the EM user to obtain statistically significant quantities of experimental data by incorporating ideas from machine learning and creating object detection algorithms. Using image processing techniques, the computer can be trained to detect microscopic features like grain boundaries, different phases, dislocations, texture, precipitates etc. which are essential for determining the structure and drawing its property correlations [5-7] .This will directly benefit the Lab's work on nanomaterials for sustainable energy conversion and storage applications, such as fuel cells and batteries.

References

1. Enhanced ionic conductivity in electroceramics by nanoscale enrichment of grain boundaries with high solute concentration. WJ Bowman, MN Kelly, GS Rohrer, CA Hernandez, PA Crozier; Nanoscale 9 (44), 17293-17302

2. Bowman et al. ACS Appl. Mater. and Interfaces (In Press)

3. https://youtu.be/2HesCYAp6H8, last accessed on November 27, 2019

4. Uusimaeki T, Wagner T, Lipinski H-G, Kaegi R (2019) AutoEM: a software for automated acquisition and analysis of nanoparticles. Journal of Nanoparticle Research, 21(6):122. https://doi.org/10.1007/s11051-019-4555-9

5. Kondrashov, D. (2018). Intelligent microscope. Eindhoven: Technische Universiteit Eindhoven.

6. Julien Maitre, Kévin Bouchard, L. Paul Bédard. Mineral grains recognition using computer vision and machine learning, Computers & Geosciences Volume 130, September 2019, Page 84

7. Modarres et al. Neural Network for Nanoscience Scanning Electron Microscope Image Recognition, Sci Rep. 2017; 7: 13282