Cornell University

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Enabling the Direct Computation of Polycrystalline Microstructures Obtained from Near-field High Energy X-ray Diffraction Microscopy (HEDM)

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Abstract

Using the near-field data obtained from the high energy X-ray diffraction microscopy (HEDM) experiments, a user-friendly graphical interface was constructed to optimize the rotational angle needed to process and prepare all data for NEPER. An angle was determined by applying a Sobel filter to the generated grain map—enhancing the grain data so edge and corner detection could occur. A 3-D mesh of the remapped microstructure was generated—enabling future work toward generating a refined mesh suitable for the crystal plasticity finite element model (CPFEM), which is essential in the comparison and validation of the simulated and reconstructed microstructures.

1 Introduction

Within the field of material science and engineering, multi-scale material modeling is an extremely difficult task. Currently, atomistic and molecular dynamical models exist, but are computationally extensive, require state of the art equipment, and are inefficient for manufacturing purposes [1]. On the larger end of the spectrum, empirical data has been collected and simulated using finite element modeling software to predict the engineering performance of materials.

The missing link, which enables designing innovative and superior materials with desired mechanical properties, is at the mesoscale. At this level, intragranular behaviors are less predictable and more complicated—increasing the complexity of a computational model [1]. Investigating a material's microstructure is important for understanding the material's internal response to an external load—this is important in reconstructing a 3-D model. With that being said, this project enables the direct computation of polycrystalline microstructures obtained from near-field high energy diffraction microscopy.

2 Background

High energy diffraction microscopy (HEDM) is an experimental technique which utilizes monochromatic x-ray beams to non-destructively investigate the micromechanical structure of a material when subjected to a mechanical load (currently uniaxial tension or compression) [2]. HEDM has both a near-field (nf) and far-field (ff) modality based on the detector placement, Figure 1.

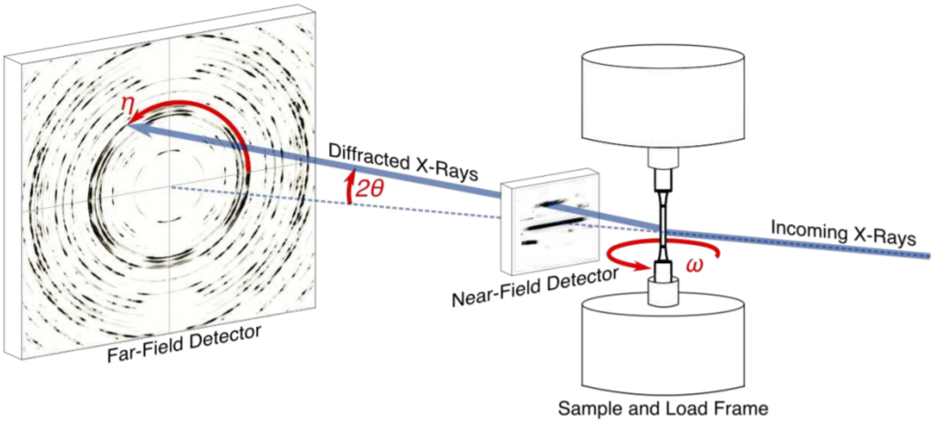

Figure 1: Experimental setup of nf- and ff-HEDM [3].

Near-field HEDM measures grain morphology and local crystallographic orientations within and between grains, while far-field HEDM measures the centroid, average elastic strain tensor, and crystallographic orientation in each individual grain [2]. By combining both techniques we can study the spatial distribution of orientation and grain morphology after loading.

3 Methodology and Results

Polycrystalline microstructures were reconstructed by utilizing far- and near- field high energy x-ray diffraction microscopy (HEDM), and subsequently tessellated and meshed using 3-D meshing software—NEPER [4]. Before using NEPER, the HEDM data array needed to be reconfigured with a new data processing step.

3.1 Preparing Near-field Data for NEPER

Figure 2 depicts a cross-sectional view of the near-field experimental data array. Successfully operating NEPER required all data to be orthogonal to the x- and y-axes. This involved determining the needed angle to straighten any skewed experimental data. Additionally, all "white" data (blue regions) were extracted and deleted.

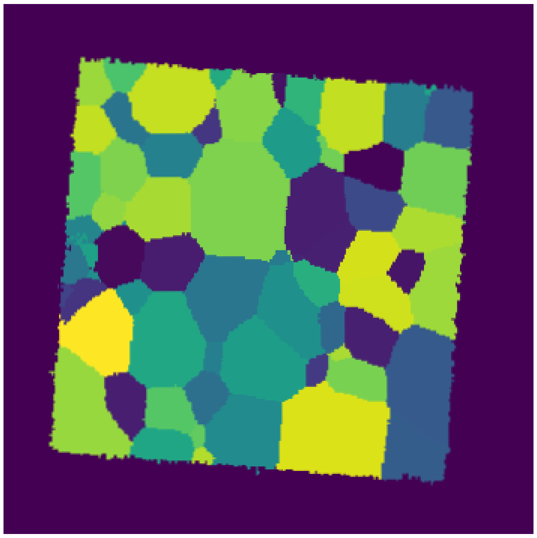

Figure 2: Cross-sectional view of the near-field data array—layer 15.

Determining the rotational angle before this project was done manually by selecting two points. Although the technique is practical, the method induces variance with every new user. This was addressed by inverting the grain map and utilizing a Sobel filter to enhance the data for edge detection, Figure 3. The Sobel filter operates by performing a 2-D spatial gradient measurement on an image. By applying two 3x3 convolution masks, edges running horizontally and vertically (relative to the image grid) are detected by approximating the gradient magnitude at each point within the image [5].

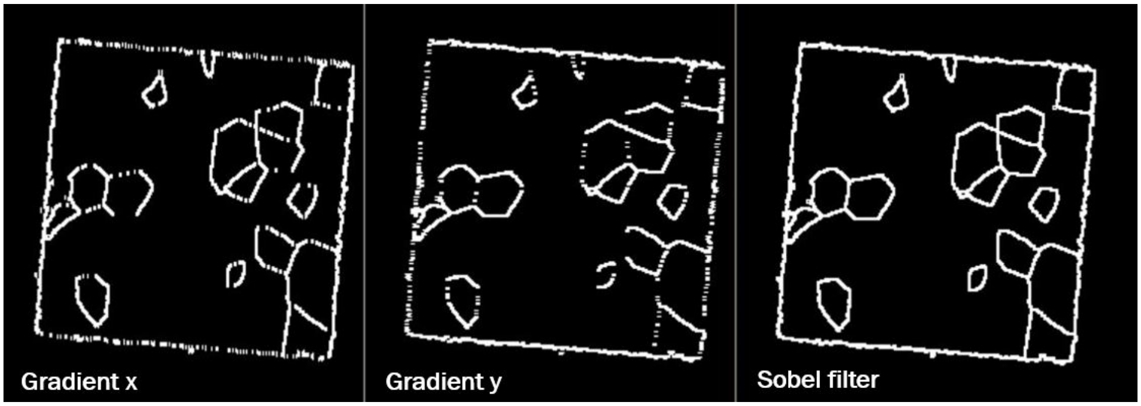

Figure 3: Utilization of the Sobel filter to enhance data for edge and corner detection.

Following the edge detection, the corners and junctions of the grain map were detected and plotted, Figure 4. Next, a user-friendly graphical interface was created—allowing the user to select any number of points within the image, which returned a list of the corresponding x- and y-coordinates relative to the size of the image. Using these points, a linear fit was applied to optimize and calculate the angle needed for rotation. This angle was used to rotate and remap the near-field data, Figure 5. This particular function also serves the added purpose of identifying grain junction points which can be used directly in data analysis and for error studies in comparison to the tessellated data. Figures 6 and 7 depict 3-D images of the remapped data using scientific visualization and data analysis tool—ParaView. Generating these images consisted of converting the near- and far-field data into a vtk file format (Visualization Toolkit).

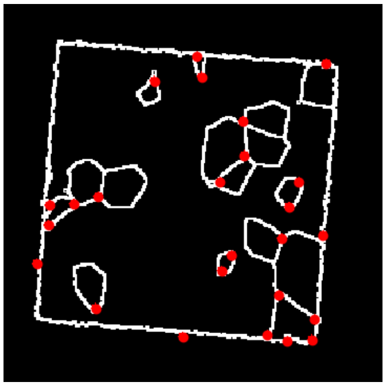

Figure 4: Corner and junction detection of individual grains.

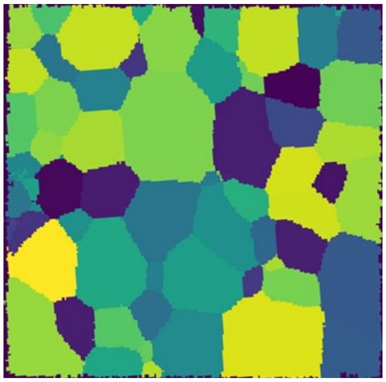

Figure 5: Rotated, translated, and remapped near-field data.

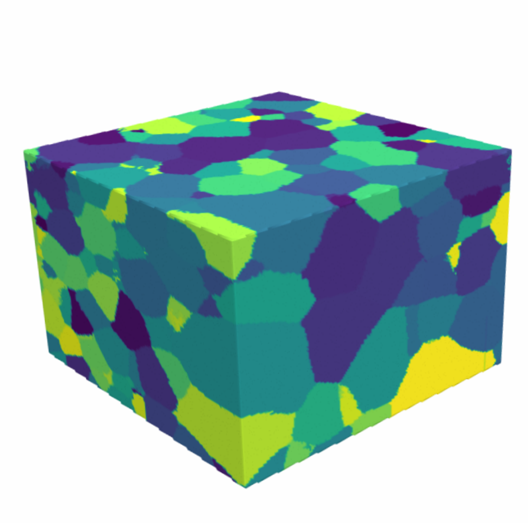

Figure 6: 3-D reconstruction of grain map using converter file and ParaView.

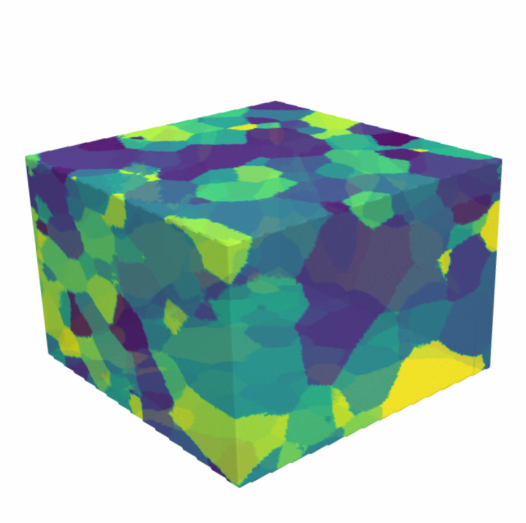

Figure 7: Transparent view of the reconstructed grain map.

3.2 Generating, Meshing, and Visualizing Microstructures in NEPER

After reconfiguring the data array, a raster tessellation file (.tesr) of the remapped data was generated specifically for NEPER. The raster tessellation file included information on the near-field data, such as the dimension, number of cells, cell identifiers, etc. Using the tesr file and NEPER modules (see NEPER code in the Appendices section), multiple 3-D visualization and tessellations of the microstructure were generated, Figures 8–11. Figure 8 visualizes the raster tessellation file, while Figure 9 shows the tessellated version using the Poisson-Voronoi tessellation method. The regularization technique was applied to the NEPER generated microstructure to remove smaller faces and edges for a better quality mesh—this technique does not effect the overall grain morphology within the microstructure [4]. Figure 10 depicts a transparent view of the 3-D tessellation, while Figure 11 highlights the edges and vertices of the first 20 grains.

By refining the tessellation processes through (a) lowering the barrier to entry by creating straight-forward processing tools and (b) increasing the fidelity of the tessellation using various techniques such as enforcing junction points and grain boundary parameters (enabled by the edge detection methods), we can begin to close the gap between the reconstructed and actual microstructures. Only by understanding these microstuctures and their internal reactions with high accuracy can we simulate their behaviors in the crystal plasticity finite element model.

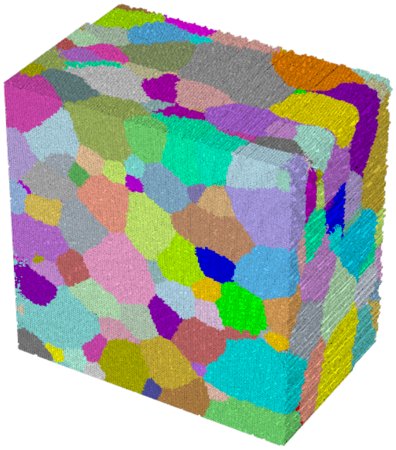

Figure 8: 3-D **visualization** of remapped near-field data in NEPER.

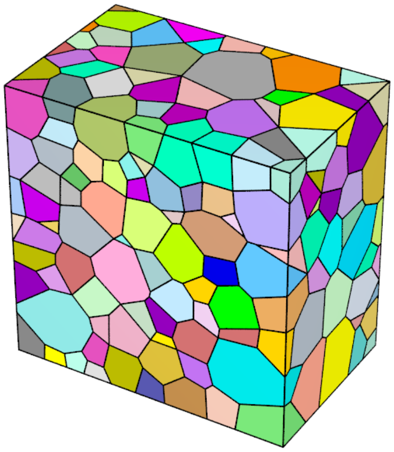

Figure 9: 3-D **tessellation** of remapped near-field

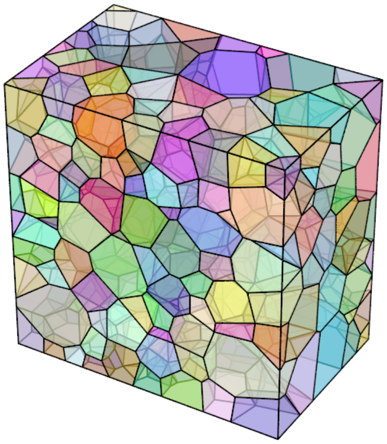

Figure 10: Transparent view of 3-D tessellation.

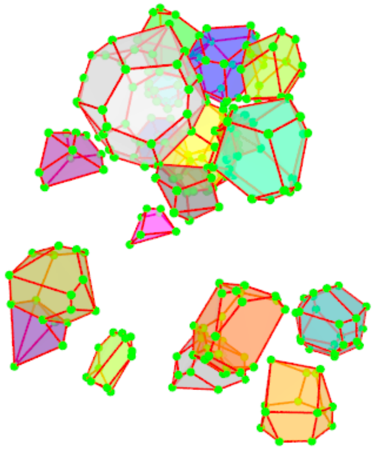

Figure 11: Edge and vertices of meshed near-field data highlighted.

4 Enabling Future Work

Within this work, the overall objective of reconstructing polycrystalline microstructures has been met, enabling future utilization of the crystal plasticity finite element model (CPFEM). This will allow users to simulate, test, and redesign materials using reconstructed microstructures.

Acknowledgements

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References

[1] R. Pokharel, *Chapter 7 Overview of High-Energy X-Ray Diffraction Microscopy (HEDM) for Mesoscale Material Characterization in Three-Dimensions*, 2018, no. September.

[2] T. J. Turner, P. A. Shade, J. V. Bernier, S. Li, J. Lind, U. Lienert, P. Kenesei, R. M. Suter, and J. Almer, "Combined near- and far-field high-energy diffraction microscopy dataset for Ti-7Al tensile specimen elastically loaded in situ," 2017.

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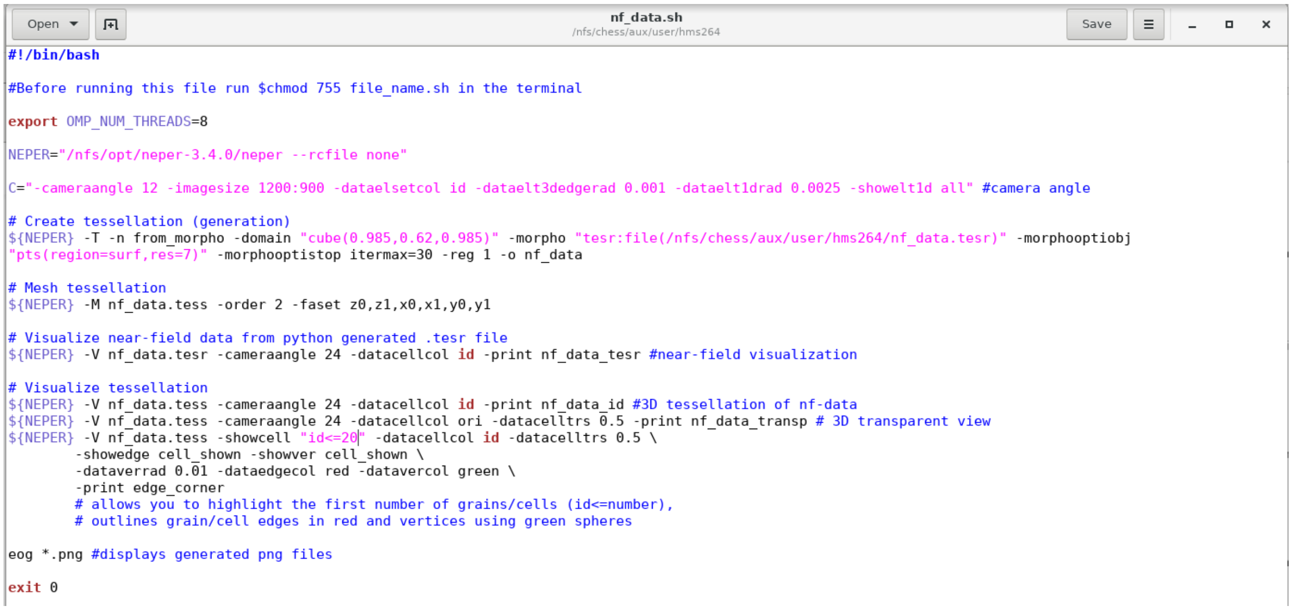
[5] S. Gupta and S. G. Mazumdar, "Sobel Edge Detection Algorithm," vol. 2, no. 2, pp. 1578–1583, 2013.

Appendices



```
#!/bin/bash

#Before running this file run $chmod 755 file_name.sh in the terminal

export OMP_NUM_THREADS=8

NEPER="/nfs/opt/neper-3.4.0/neper --rcfile none"

C="-cameraangle 12 -imagesize 1200:900 -dataelsetcol id -dataelt3dedgerad 0.001 -dataelt1drad 0.0025 -showelt1d all" #camera angle

# Create tessellation (generation)
${NEPER} -T -n from_morpho -domain "cube(0.985,0.62,0.985)" -morpho "tesr:file(/nfs/chess/aux/user/hms264/nf_data.tesr)" -morphooptiobj
"pts(region=surf,res=7)" -morphooptistop itermax=30 -reg 1 -o nf_data

# Mesh tessellation
${NEPER} -M nf_data.tess -order 2 -faset z0,z1,x0,x1,y0,y1

# Visualize near-field data from python generated .tesr file
${NEPER} -V nf_data.tesr -cameraangle 24 -datacellcol id -print nf_data_tesr #near-field visualization

# Visualize tessellation
${NEPER} -V nf_data.tess -cameraangle 24 -datacellcol id -print nf_data_id #3D tessellation of nf-data
${NEPER} -V nf_data.tess -cameraangle 24 -datacellcol ori -datacelltrs 0.5 -print nf_data_transp # 3D transparent view
${NEPER} -V nf_data.tess -showcell "id<=20" -datacellcol id -datacelltrs 0.5 \
        -showedge cell_shown -showver cell_shown \
        -dataverrad 0.01 -dataedgecol red -datavercol green \
        -print edge_corner
        # allows you to highlight the first number of grains/cells (id<=number),
        # outlines grain/cell edges in red and vertices using green spheres

eog *.png #displays generated png files

exit 0
```

Figure 12: NEPER code used to generate 3D mesh visualization and tessellations.