Advanced Image Processing Methods for Automated Quantitative Microstructural Analysis

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Recommended Citation
Advanced Image Processing Methods for Automated Quantitative Microstructural Analysis

A Thesis

Presented to the Faculty

of the Department of Mathematics and Computer Science

McAnulty College and Graduate School of Liberal Arts

Duquesne University

in partial fulfillment of

the requirements for the degree of

Masters of Science in Computational Mathematics

by

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April 3, 2006
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Advanced Image Processing Methods for Automated Quantitative Microstructural Analysis

Master of Science in Computational Mathematics

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Chapter 1

Introduction

Nonlinear algorithms have become commonplace in the field of image processing during the past 15 years. However, most applications of image processing outside the field have not taken advantage of these recent algorithms. The purpose of this project is to investigate and analyze the application of anisotropic nonlinear image processing techniques to problems in the area of microstructural analysis.

1.1 Microstructural Analysis

The physical properties of a material can be assessed and optimized via the study of its microstructural behavior. The following work will study crystalline materials, which are materials composed of microscopic crystals or 'grains'. Their basic features such as the length of grain boundaries and
the angles of grain intersections are obtained from a transmission electron microscope (see Figure 1.1). These features give insight into the behavior of the material.

Transmission electron microscopy produces images differently than a common optical based microscope. Electrons pass through a thin film of target material and are diffracted based upon the orientation of the material grains. In order to aid in the boundary detection process, a single field of view must be imaged at several different tilts. The different angles produce images of the same field of view, but often highlighting different grain boundaries. The composite of the boundaries obtained from the different tilts contains the majority of boundaries in the field of view and serves to minimize the number of false positives.

Large datasets of boundaries (on the order of thousands of grains) are required to infer meaningful information about a material. Currently the only reliable way to accomplish this task is for experts to hand trace the grain boundaries and verify the results. Therefore, much human effort is required to produce reliable results. Automation of this task would greatly improve the ability of researchers to analyze microstructural features and optimize materials for use in a variety of real world applications, from aircraft manufacturing to microprocessor production.
Figure 1.1: Transmission Electron Microscope (TEM) images of a sample of aluminum taken at four different tilt angles (All images in this work courtesy of K. Barmak, Department of Material Science Engineering, Carnegie Mellon University).
1.2 Related Work

Previous attempts at automation of grain boundary detection used mostly standard image processing techniques [CRB98]. The automated methodology showed promise; however, its success was greatly dependent upon images that were highly optimized for the study. These images required a great deal of human effort to generate, thus reducing the benefit of automating the boundary detection process.

In general, the TEM process produces images that are not easily compatible with standard image processing techniques. The images in Figure 1 demonstrate some of the issues encountered with TEM images. Certain aperture settings of the microscope can produce images with poor contrast, leaving many grain boundaries imperceptible. Other aperture settings of the TEM produce higher contrast images which preserve more grain boundaries. Unfortunately, these higher contrast images often have 'shadows' internal to a grain due to the grain’s physical orientation. These 'shadows' can appear as false grain boundaries.

To overcome these limitations inherent in the TEM process, each field of view is imaged four times at slightly different angles. The redundancy often provides enough information for the human eye to determine which contrast variations are due to grain boundaries, and which are artifacts due to grain orientation. The current state of the art is for an expert to hand trace the grain boundaries of four tilts of a given field of view from which a composite
grain boundary map is made. A second expert is then required to verify these results, making data collection a prohibitively laborious process. This work seeks to develop a methodology that will automate part or (ideally) all of this process.
Chapter 2

Methodology

An algorithm for grain boundary detection composed of a series of image processing techniques is proposed in this thesis. The algorithm consists of seven steps: noise removal, edge detection, registration of edge sets, thresholding, connecting broken edges, thinning, and pruning the final boundaries.

2.1 Noise Removal

TEM images have some level of noise due to inhomogeneities in the material or noise acquired through the imaging equipment. Standard approaches to noise removal typically make use of a linear, isotropic, Gaussian-type filter, or a median filter. Linear filters often blur object boundaries (Fig. 2.1 (c)), while median filters can shift boundaries or introduce false ones (Fig. 2.1 (d)).
Linear low pass filters are often implemented as a convolution of a kernel (a small matrix) with the image. The kernel generates a weighted average of neighboring intensity values to replace each pixel value. Linear filters such as the Gaussian diffuse isotropically, i.e. equally in all directions. They use a convolution mask where the largest weight is in the middle and the values decrease equally in all directions as the distance from the center pixel increases. While noise is reduced, important features are also blurred. This loss of information is detrimental to methods that occur after the noise removal process since 'edges' or 'object boundaries' are not preserved; this is especially true if a large amount of smoothing is required to reduce the amount of noise in the image (see Figure 2.1 (c)).

Median filters replace each pixel value in an image with the median of the surrounding pixels. Typically, a window of size 3×3, 5×5, or 7×7 is used for median filtering. This method works extremely well with "salt-and-pepper" noise; however, the median filter has more trouble on images with Gaussian noise. It also performs poorly on images with large amounts of noise since the median value of a given window will likely contain noise rather than meaningful information (see Figure 2.1 (d)).

Nonlinear diffusion based models remove noise by averaging image intensities anisotropically, that is, the averaging favors a certain direction. For example, the averaging can be tuned so it favors the direction tangential to edges. The goal is that this 'weighted' smoothing will be done in a manner that preserves important features of the original image.
Two anisotropic models have shown promise for the noise removal step. The first model is based on minimizing the total variation (TV) of the image \cite{ROF92}. The second is a model that combines TV minimization and isotropic smoothing.

The total variation of an image is computed by summing all of the intensity changes within the image. This TV minimization problem attempts to reduce the amount of changes in an image, while preserving the mean of the original image. In the continuous setting, the total variation model \cite{ROF92} is defined as

\[ TV(u) = \int_{\Omega} |\nabla u| \, dx \]

subject to

\[ \int_{\Omega} u \, dx \, dy = \int_{\Omega} u_0 \, dx \, dy, \text{ where } u_0 \text{ is the initial image.} \]

One can show that the TV model preserves edges by averaging pixels in a direction tangential to likely edge locations; using the tangential direction prevents the loss of information by not smoothing across edges (Fig. 2.1 (e)). Minimizing the total variation yields a piecewise constant image; this works well on low contrast grain images as we will see in chapter 3. However, as the variation in the image increases, smooth gradients will be replaced with a piecewise gradient made up of a series of bands or steps. This gradient introduces artificial edges that appear in later steps. Notice the 'steps' across
the gradient filled square in (Fig. 2.1 (e)). In the grain boundary problem, these artificial edges are most evident in high contrast images.

An adaptive model can be used to deal with the problem of artificial edges [CLR05]. The model uses the total variation method near potential edges in order to preserve them. However, away from edges the model uses isotropic diffusion to smooth in all directions. Notice how well the model performs across the gradient filled square in comparison to the total variation model (Fig. 2.1 (f)). Thus, edges are preserved while false boundaries inside of a grain are suppressed.

### 2.2 Edge Detection

After noise removal, an edge detector is run on the reconstructed image. Standard edge detectors are often linear operators that work off of limited information. A Sobel filter is an example of a linear edge detector (Fig. 2.2 (b)). The Sobel filter attempts to measure the magnitude of the gradient to determine areas of changing intensity. Another commonly used edge detector is the Laplacian (Fig. 2.2 (c)). The Laplacian uses the second derivatives of the image to determine areas of changing intensity.

In this work, a nonlinear edge detector based on the magnitude of the gradient is used [PM90]. This edge detector function $g$ is defined as

$$g(\nabla u) = e^{-\left(\frac{\|\nabla u\|}{K}\right)^2},$$

where $K \in \mathbb{R}^+$ is given.
Figure 2.1: Noise removal methods: (a) Original image. (b) Image with random noise. (c) Gaussian. (d) Median. (e) Total variation. (f) Adaptive model.
The change of intensity around a pixel is measured by the gradient. A larger change in intensity represents greater likelihood that the pixel lays on an edge. The nonlinear edge detector can produce a more accurate edge map by adjusting the constant $K$ and taking more local information into account (Fig. 2.2 (d)).

### 2.3 Registration

At this point in the process, noise has been removed and the edges identified for each of the individual images for a given field of view. Next, we produce a single composite edge map of likely grain boundaries from the edge maps of the individual images via a registration process using a standard cross correlation method which minimizes the difference between the pixel values of the images, thus producing the best aligned image. Two images with similar features (Fig. 2.3 (a) and Fig. 2.3 (b)) are combined so as to align similarly valued pixels (Fig. 2.3 (c)).
Thresholding converts the grayscale edge maps into a binary image. Standard thresholding converts all values above a certain threshold to white pixels, and all values below a certain threshold to black pixels. In the grain boundary problem, the edge map often contains many false edges or boundaries due to variations within individual grains. Therefore, standard thresholding methods would produce a binary image with both true and false edges. A less aggressive threshold value must be used to reduce the amount of false boundaries detected (Fig. 2.4 (b)). In order to avoid this situation, a double thresholding method is used (Fig. 2.4 (c)) [Rus99].

First, the image is thresholded at a very low value. This produces an image with very few black pixels. These few black pixels are assumed to definitely be part of edges. The image is then thresholded at a higher value. This second thresholded image contains black pixels that are due to noise as well as real edges. At this point, all black pixels in the second thresholded
image that are not connected to black pixels in the first image are removed which preserves edges while removing any artifacts not connected to edges. One drawback is that any noise connected to an edge will be preserved; however, this is still an improvement over a standard single thresholding method.

## 2.5 Dilation

Two dilation models were investigated. The first model is standard dilation. The features of the image are expanded isotropically in the image. This is accomplished by activating the pixels surrounding the currently active pixels. Regular dilation can destroy fine features in the image because it thickens boundaries (Fig. 2.5 (b)). The other method investigated was coherence-enhancing anisotropic diffusion [Wei95, GRV03]. Like the noise removal models above, this method diffuses in a direction tangential to likely object boundaries.
The anisotropic this method only diffuses on the likely boundaries, which results in an extension of the boundaries to close small gaps without increasing the boundary thickness (Fig. 2.5 (c)). In the current algorithm, the regular dilation performed better than the coherence-enhancing diffusion. This was mainly due to two factors. First, regular dilation ’swallows’ spurious details and connects misaligned edges. Second, many of the gaps along the grain boundaries were too large for the anisotropic method to connect.

### 2.6 Skeletonization

The focus now turns to skeletonization of the grain boundaries. After the image of likely edges is thresholded, the grain boundaries are skeletonized [Rus99]. The method reduces the image to a binary image made up of pixel wide segments, while preserving topology and angles between the segments. The image is successively thinned until all segments are a single pixel wide;
this process is done in such a way that no pixels are removed that would modify the topology of the boundaries (Fig. 2.6 (b)). Skeletonization is used in place of a standard erosion method that can move edges or cause 'breaks' in the boundaries. At this point, the image consists of pixel wide boundaries and spurs.

![Skeletonization](image)

(a) (b)

Figure 2.6: Skeletonization: (a) Dilated image. (b) Skeletonized image.

### 2.7 Pruning

The image now consists of pixel wide segments; some of these segments form simple closed curves. Pruning is an iterative process that shortens all segments which do not form simple closed curves; this converges to an image that only contains simple closed curves (Fig. 2.7 (b)). In this problem domain, the simple closed curves that remain are the potential grain boundaries.
2.8 Post Processing

Upon completion of the process, the image consisting of pixel wide grain boundaries can be used as input to standard image analysis software (e.g. NIH image). Properties such as grain size and shape can then be measured and finally used to infer important information about the material. The success of the new method will be measured by comparison of the grain diameters detected by the proposed method to those detected by hand tracing the grain images.
Chapter 3

Results

Figure 3.1: Image sets: (a) Optimized Bright Field. (b) Unoptimized Bright Field Negative.

Two different sets of TEM images have been analyzed with the above methodology. The first set of images is a set of optimized 'bright field’ images of aluminum grains. This set of images consists of low contrast,
mostly homogenous grains. While variation exists within individual grains, it is usually limited in magnitude (Fig. 3.1 (a)). The second set of images is a series of unoptimized bright field image negatives of aluminum grains. This set of images is characterized by high contrast, including significant variation within individual grains (Fig. 3.1 (b)).

### 3.1 Bright Field Images

In general, the bright field images (Fig. 3.2) yielded much better results. The limited variation within individual grains allowed for a more aggressive edge detection mechanism. During the noise removal step, most grains were successfully reduced to homogenous regions (Fig. 3.3) as seen in the edge maps produced from the smoothed images (Fig. 3.4). Upon registration, the edges from each of the individual images produce a fairly complete edge map (Fig. 3.5). Thresholding isolated the strongest potential edges (Fig. 3.6), while dilation connected incomplete boundaries (Fig. 3.7). Skeletonization (Fig. 3.8) and pruning (Fig. 3.9) produced a large number of reliable grain boundaries. The final boundaries from the process can be seen overlaid on the original image (Fig. 3.10). Figure 3.11 shows the final boundaries from another set of bright field images.

Additionally, the bright field images were compared to hand traced grain boundaries. Hand tracings for this set of images were not available. Thus, hand tracings from the bright field negatives were used. The images are of
Figure 3.2: Bright field TEM images of aluminum grains
Figure 3.3: Bright field images after adaptive noise removal step
Figure 3.4: Bright field images after edge detection
Figure 3.5: Registered edge maps of bright field images
Figure 3.6: Bright field images after double thresholding
Figure 3.7: Bright field images after dilation
Figure 3.8: Bright field images after skeletonization
Figure 3.9: Final grain boundaries of bright field images
Figure 3.10: Final grain boundaries of bright field images overlaid on original image
Figure 3.11: Final grain boundaries of a different set of bright field images overlaid on original image
the same material (aluminum), and thus the grain size distribution should be comparable. The grain sizes were normalized to the largest detected grain size, since the scales of the two image sets could not be ascertained. Thus, grain sizes are shown as a percent in terms of the largest grain size. The lower sizes are shown individually, while larger sizes are grouped since they occur much less frequently. Figure 3.12 shows the amount of grains of each size as a percent of the total number of grains. Grains that are approximately three percent the size of the largest grain make up approximately twelve percent of hand-traced grains and approximately eleven percent of automated grains. The chart shows that the distribution of grain sizes from the automated process correspond well to those acquired through hand tracing.

3.2 Bright Field Negatives

The bright field negatives proved more challenging than the bright field images. The amount of variation within the grains (Fig. 3.13) introduced false boundaries, even with a very relaxed edge detection scheme (Fig. 3.14 (b)). The conservative edge detection scheme which was used leaves many edges undetected. Even after registration, the grains are often incomplete (Fig. 3.15). Potential edges are conserved throughout thresholding (Fig. 3.16), dilation (Fig. 3.17), and skeletonization (Fig. 3.18). If the registered edge maps are reduced to a subset that only contains simple closed curves, no grains are accurately represented (Fig. 3.19). However, a more limited
Figure 3.12: Comparison of automated grain detection to hand tracings for low contrast images.
amount of pruning may be performed to only remove spurious details (Fig. 3.20). The limited pruning results in a set of boundaries that could be useful as a starting point for hand tracing (Fig. 3.21).

Figure 3.13: TEM bright field negatives of aluminum grains

Figure 3.14: Edge maps of bright field negatives
Figure 3.15: Registered edge maps of bright field negatives
Figure 3.16: Bright field negatives after double thresholding
Figure 3.17: Bright field negatives after dilation
Figure 3.18: Bright field negatives after skeletonization
Figure 3.19: Bright field negatives after pruning
Figure 3.20: Bright field negatives after limited pruning
Figure 3.21: Bright field negatives after limited pruning overlaid on original image
In conclusion, this thesis introduces a method for automated grain boundary detection. The method operates on general unoptimized TEM images, which removes the requirement of large amounts of human intervention needed in previous attempts at automation. The bright field images yielded impressive results, even with a fully automated algorithm. The algorithm performed very well in comparison to hand traced grain boundaries which allows for large sets of images to be automatically processed. The bright field negatives yielded less positive results than the bright field images. The contrast variations within the grains often exceeded the contrast variation at grain boundaries. This posed great problems within this methodology. However, if limited pruning is used the algorithm can produce a good starting point for hand tracing the images.
Bibliography


