Analyzing Grain Boundaries Using Gabor Filters and K-means Clustering

A. Hernandez-Robles, B. Paniagua, and A. Ponce

Department of Physics and Astronomy, University of Texas at San Antonio, San Antonio, Texas, 78249, United States.

Abstract

This study investigates the use of Gabor filters and K-means clustering to extract crystallographic data from TEM images of materials having grain boundaries. The purpose is to effectively identify faults and generate crystal orientation maps. Gabor filters are used to identify abrupt changes in intensity, and K-means clustering is utilized to uncover patterns in the recovered features. The results suggest that this method can detect flaws and extract considerable crystallographic information, making it a valuable tool for future materials research.

Introduction

- Nanomaterials exhibit distinct features when compared to ordinary materials and have been the subject of substantial research in recent decades [1].
- With the use of TEM imaging, particle segmentation is employed to analyze the grain boundaries of nanoparticles.
- Here we use Gabor filters for feature extraction and unsupervised learning in image segmentation on grain boundaries.
- New nanoscale analysis technique advances knowledge of nanomaterials without experimental or model-based learning.

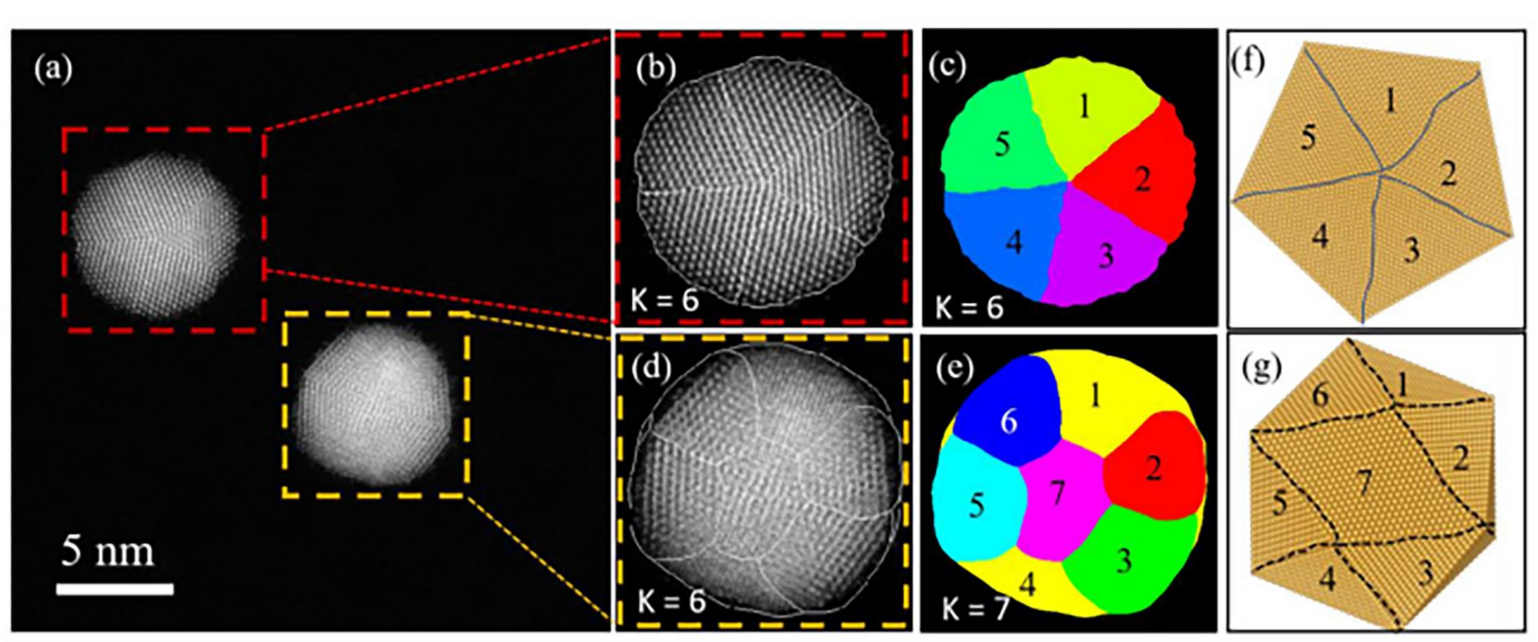

Figure 1: *a) Segmentation of two particles through b) skeletonization, c) cluster coloring, and d) facet delimitation. Source: Guillermo Barcena-Gonzalez et al. [2]*

Methods

- Gabor filters efficiently extract features with K-means clustering making them suitable for evaluating crystalline materials [2][3].

Gabor feature extraction MATLAB code

Extracts the Gabor features of an input image. It creates a column vector, consisting of the Gabor features of the input image.

```
function featureVector = gaborFeatures(img,gaborArray,d1,d2)
% GABORFEATURES extracts the Gabor features of an input image.
%
% Inputs:
%       img          :   Matrix of the input image
%       gaborArray   :   Gabor filters bank created by the function gaborFilterBank
%       d1           :   The factor of downsampling along rows.
%       d2           :   The factor of downsampling along columns.
%
% Output:
%       featureVector   :   A column vector with length (m*n*u*v)/(d1*d2).
%                           This vector is the Gabor feature vector of an
%                           m by n image. u is the number of scales and
%                           v is the number of orientations in 'gaborArray'.

img = imread('sample.tif');

% Generates the Gabor filter bank
gaborArray = gaborFilterBank(5,8,39,39);

% Extracts Gabor feature vector, 'featureVector', from the image, 'img'.
featureVector = gaborFeatures(img,gaborArray,4,4);
img = double(img);


% Filter the image using the Gabor filter bank
% Filter input image by each Gabor filter
[u,v] = size(gaborArray);
gaborResult = cell(u,v);
for i = 1:u
    for j = 1:v
        gaborResult{i,j} = imfilter(img, gaborArray{i,j});
    end
end

% Extract feature vector from input image
featureVector = [];
for i = 1:u
    for j = 1:v

        gaborAbs = abs(gaborResult{i,j});
        gaborAbs = downsample(gaborAbs,d1);
        gaborAbs = downsample(gaborAbs.',d2);
        gaborAbs = gaborAbs(:);

        % Normalized to zero mean and unit variance.
        gaborAbs = (gaborAbs-mean(gaborAbs))/std(gaborAbs,1);

        featureVector =  [featureVector; gaborAbs]; %#ok<*AGROW>

    end
end
```

K-means MATLAB code

The function assumes each data point is stored in a row. Therefore, data is expected to have N rows and M columns, and K is an integer greater than 1

```
function centroids=kmeans(data,K)
% KMEANS – K-means algorithm
%
%    data      : NxM data matrix of N points with M characteristics
%    K         : desired number of centroids
%    centroids : KxM matrix of K points with M characteristics


% 1. Choose random initial centroids
choice      = randperm(size(data,1),K);
centroids   = data(choice,:);
oldcentroids = zeros(size(centroids));

% 2. Loop
it = 1;
while (sumsqr(oldcentroids-centroids)>1e-6) && (it<30)

 oldcentroids = centroids;

 % 2a. Calculate closest centroid to each data point
 for i=1:K
  d(:,i) = pdist2(data,centroids(i,:));
 end
 [~,class]=min(d,[],2);

 % 2b. Recalculate centroids
 for i=1:K
  centroids(i,:)=mean(data(class==i,:));
 end

 % Increase loop index
 it = it + 1;

end
```

Results

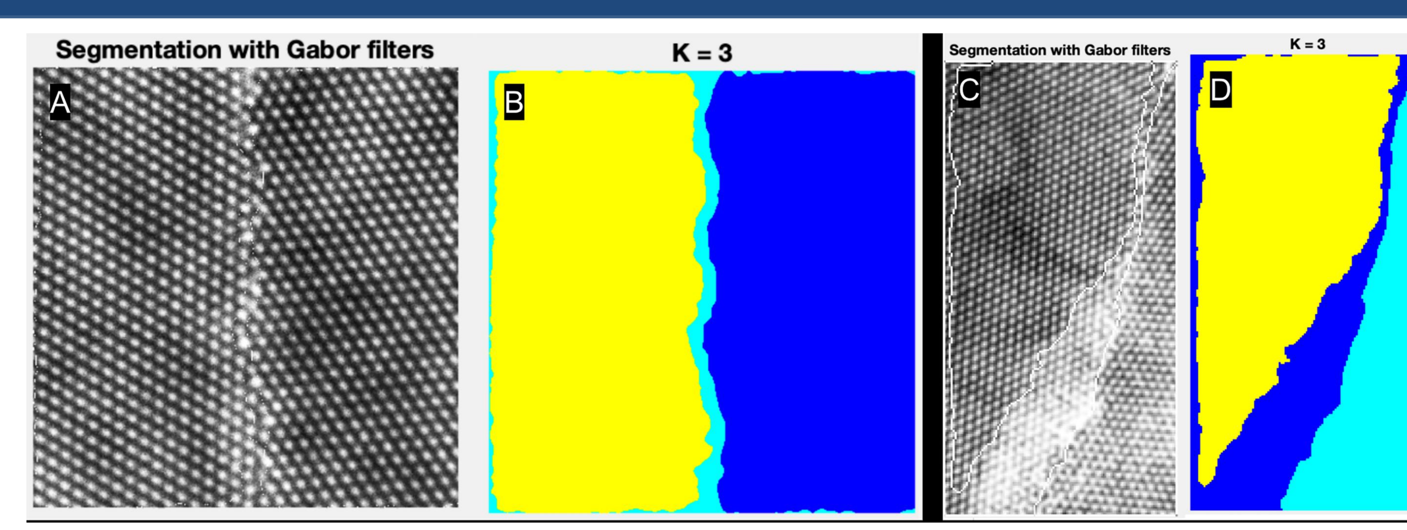

Figure 3: *Two ZnO grain boundaries a) type sigma 7 b) colorization of (a), c) sigma 13*

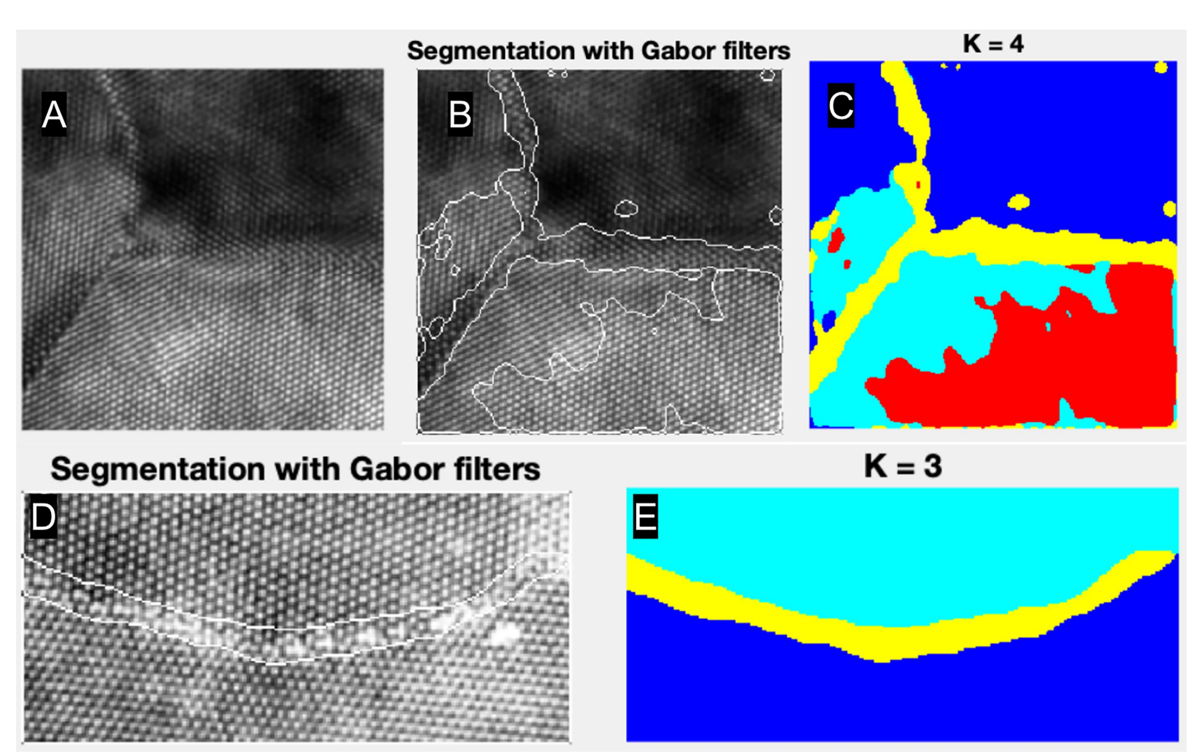

Figure 4: *ZnO sigma 13 grain boundaries A) three crystals , D) two crystals*

Summary

- Here we utilize Gabor filters and unsupervised learning to perform particle segmentation on nanoparticle crystalline grain boundaries.
- Testing on cross-sections of ZnO particles demonstrated the segmentation algorithm's effectiveness in identifying grain boundaries and crystal facets within complex microstructures.
- Initial parameter fine-tuning is required for the technique, but implementing advanced deep learning techniques can automate this process and improve accuracy.
- Developing a dependable and precise technique for segmenting crystalline nanoparticles holds practical significance for materials science and nanotechnology.

References

1. H. Gleiter, B. Chalmers, Progress in mater, Sci 33 (1989) 223.
2. G. Barcena-Gonz ´ alez, A. Hern ´ andez-Robles, ´ A. Mayoral, L. Martinez, ´Y. Huttel, P. L. Galindo, A. Ponce, Unsupervised learning for the segmentation of small crystalline particles at the atomic level, Crystal Research and Technology (2022) 2200211.
3. J. Delua, Supervised vs. unsupervised learning: What's the difference?(Mar 2021).
4. M. Haghighat, S. Zonouz, M. Abdel-Mottaleb, Cloudid: Trustworthy cloud-based and cross-enterprise biometric identification, Expert Systems with Applications 42 (2015) 7905–7916.

Acknowledgements

I thank Arturo Ponce and Andrei Hernandez-Robles for their guidance on this project. A special thanks to Andrei Hernandez-Robles for providing key information and supplying all the HRTEM samples used. Their contributions were invaluable to enhancing the visual appeal and scientific accuracy of the research poster.