Detection of Disk-Like Particles in Electron Microscopy Images

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Abstract. Quantitative and qualitative description of particles is one of the most important tasks in the Electron Microscopy (EM) analysis. In this paper, we present an algorithm for identifying ball-like nanostructures of gahnite in the Transmission Electron Microscopy (TEM) images. Our solution is based on the cross-entropy clustering which allows to count and measure disk-like objects which are not necessary disjoint or with not smooth borders.

1 Introduction

In the recent years, describing the structure of nanomaterials with measure from a few to several hundred nanometers become very important in particular in medicine and biology [3, 4, 9]. Ball-shaped nanoparticles of gahnite with a biologically active layer adsorbed to their surface have the potential to be used as a biological nanosensors [6, 13]. The geometry and the size of a gahnite nanoparticle is very important as is determines its ability to be injected into blood vessel as biological nanosensor. One of the most important and most reliable techniques for identifying the nature and form of nanomaterials is Transmission Electron Microscopy (TEM). In the case of gahnite nanoballs, the quality of nanomaterial produced depend on the number and size of ball-like nanoparticles.

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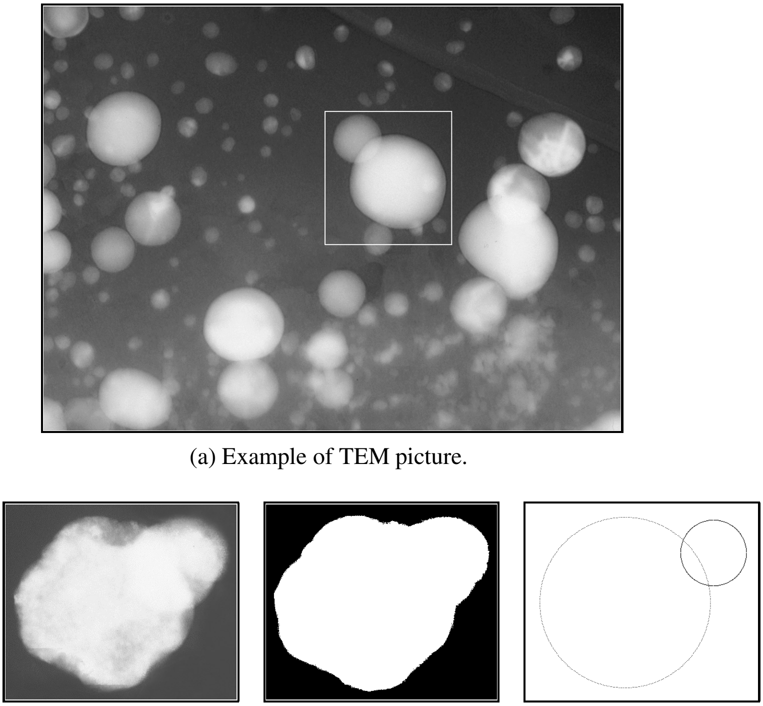
* The work of this author was supported by the European Regional Development Fund within the Innovative Economy Operational Programme 2007-2013 (UDA–POIG.01.03.01-14-071/08-07).

R. Burduk et al. (Eds.): *CORES 2013*, AISC 226, pp. 411–417.
DOI: 10.1007/978-3-319-00969-8_40



(a) Example of TEM picture.

(b) The original dataset. (c) The image after thresholding. (d) Circles detected by CEC.

Fig. 1 The results of the CEC algorithm

In this paper we present a method for estimating the number and size of the gahnite nanoballs that are observed in TEM images. The nanomaterial analyzed consists of nanocrystalline structures and amorphous substance. The amorphous substance, as shown in Fig. 1, and not completely regular shapes of "nanoball" (2) imply that the standard image processing techniques, which use the Hough Transform (HT) [1, 5, 7, 14], are not sufficient. The basic idea of HT circle detection is based on analyzing edges in images. However, in our case objects in the picture do not have smooth borders and in many cases the "circles" are not disjoint (Fig. 1a) which causes difficulties in determining edges.

On the other hand, due to various types of image deformation caused by specific construction of tested materials and measurement inaccuracies, nanocrystals (similar to 3D balls) sometimes do not look like disks in images. In such cases, the circle is deformed and looks like an ellipse. Moreover, we have to deal with the noise that makes it difficult to analyze images. Fig. 1a presents examples of the TEM pictures.

This paper presents a method based on the cross-entropy clustering [11] (CEC) instead of HT. This method has a few advantages over the standard approach. First of all, we do not need to extract edges. Instead of this we apply simple thresholding based on the Otsu algorithm [8]. Moreover, we can find elements which are not exactly a disc. The results of our investigation can be applied in the case of nanomaterials with nanoparticles with approximately spherical shapes.

Let us discuss the contents of this paper. In the first part of our work we briefly describe the CEC algorithm and present its advantages and disadvantages in the context of disks detection (in the case of TEM images). In the third section we present practical implementation of our approach.

2 CEC Approach to Circle Detection

In this section we give a short introduction to Spherical CEC[2] in the case of disks detection, for more detailed explanation we refer the reader to [11]. Let $Y = \{y_1, \dots, y_n\}$ be arbitrary given dataset[3]. Our goal is to split the data set into k disjoint subsets $Y_1, \dots, Y_k$ (the number of groups is unknown), such that each cluster is well approximated by a disc. Spherical cross–entropy clustering divides the dataset into groups by trying to minimize the "energy function" given by:

$$E((Y_i)_{i=1}^k) = \sum_{i=1}^{k} p(Y_i) \cdot [\tfrac{N}{2} \ln(2\pi e/N) - \ln(p(Y_i)) + \tfrac{N}{2} \ln(\mathrm{Tr}(\Sigma_{Y_i}))], \qquad (1)$$

where $p(Y_i) = \mathrm{card}(Y_i)/\mathrm{card}(Y)$ denotes the probability of choosing Y_i, Σ_{Y_i} is covariance matrix of Y_i and m_{Y_i} denotes the mean of Y_i.

Since CEC is a generalization of the classical k-means method we use Hartigans approach to minimize equation (1). Full description of the algorithm can be found in [11]. The most powerful properties of this method is that it simultaneously deletes unnecessary clusters and is scale invariant, that is it well detects disks of various sizes.

In the case of a set containing k disjoint circles (in $\mathbb{R}^2$), we obtain k clusters containing them where each of group is described by the mean and covariance matrix. Making use of [11], one can deduce the following properties of spherical CEC:

- Let a set $Y \subset \mathbb{R}^2$ be the sum of $k \in \mathbb{N}$ disjoint disks $Y_1, \dots, Y_k$. Then for any other division $\bar{Y}_1, \dots \bar{Y}_k$ of Y we have:

$$E((\bar{Y}_i)_{i=1}^k) > E((Y_i)_{i=1}^k).$$

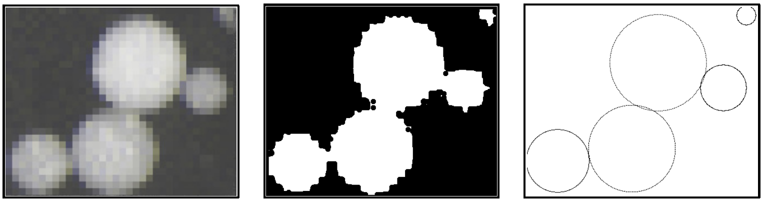
- Let $Y \subset \mathbb{R}^2$ be a disc–like dataset.Then the optimal disc describing Y is approximately given by

$$Y \approx \mathscr{B}(\mathrm{m}_Y, \sqrt{2\mathrm{Tr}(\Sigma_Y)}).$$

As was mentioned earlier, in the case of a TEM picture we need to deal with shapes which are not exactly disks (see Fig. 1(b)). The second problem with the TEM

[2] Since we use only the Spherical version of CEC, we will use abbreviation CEC to denote Spherical CEC.

[3] In our case the set of coordinates of pixels which are inside circles in the picture.



(a) The original dataset. (b) The image after thresholding. (c) Circles detected by CEC.

Fig. 2 The results of the CEC algorithm

pictures is that edges can be not smooth (Fig. 4a). In fact, this is another reason why we can not easily use the HT method to analyze this kind of images. Instead of edge detection, CEC use thresholding which is simpler and needs fewer parameters. Fig. 2(c) presents the results of the CEC algorithm in such a case.

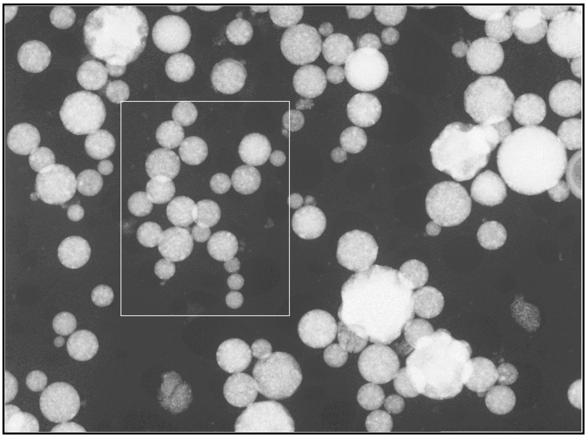
As we see, in our case the shape of edges is not as important as in the classical methods. Since CEC is resistant to low distortion of the set, we can even radically shrink the image before the algorithm is started (Fig. 2a). Even in this situation, CEC detects clusters correctly. A smaller version of the image does not contains all pixels from the original one, so small circles can disappear. Nevertheless, the operation described allows us to cluster the whole picture quickly.

3 Description of the Algorithm

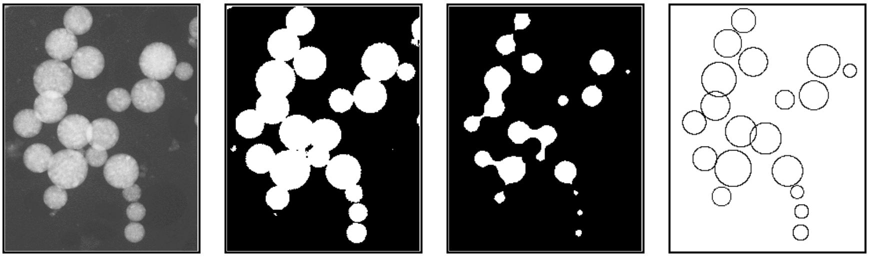
In this section, we present a detailed description of proposed algorithm. As was mentioned earlier, CEC works on a binarized version of images, therefore we begin by thresholding by the Otsu algorithm [8].

In a natural way, thresholding has a great influence on the final algorithm results. In some situations it causes disappearing of small circles (which are interpreted as elements of the background) or deforming of existing one (by adding background elements). As we mentioned earlier, our method copes well with such set distortion and not disjoint disks. Nevertheless, CEC gives better results if analyzed shapes are disjoint disks. Therefore, we use a morphology operation [10, 12], namely erosion. Thanks to this, we obtain splitting the dataset into small connected components which contains more separated elements. Erosion gives a good effect in the cases of a picture containing groups of circles which are not disjoint. We present this kind of a picture in Fig. 3. This modification divides the set and extracts circles. After erosion, the circles radius are smaller then this on the original picture. The resizing depends on a structural element used in erosion.

In the next step, we divide the picture into connected components. This allows us to work with smaller amounts of data. In many cases we obtain groups containing only a few disks, where CEC works fast sufficiently. After division we apply CEC to each component.



(a) Example of TEM picture.



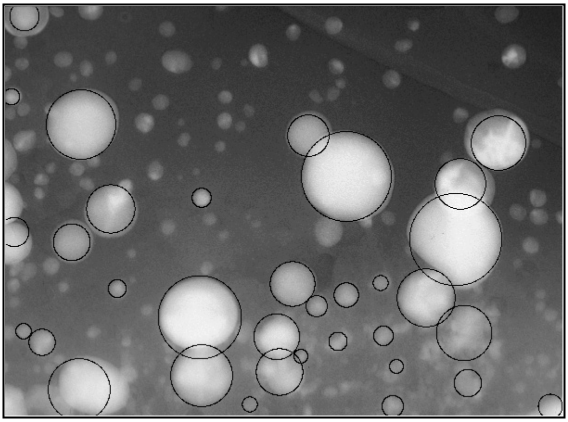
(b) The original dataset. (c) The binarizatoin of the image. (d) The image after erosion. (e) Circles detected by the CEC algorithm.

Fig. 3 The results of the CEC algorithm with radius corrected respectively to the structural element which was used in erosion

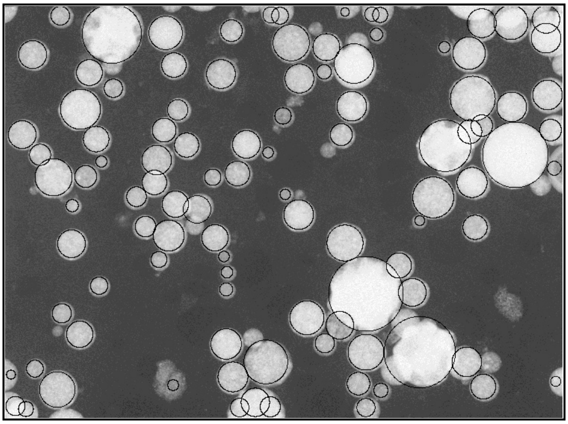
Our method gives good results in most of the cases, nevertheless we are not able to detect circles that are not fully in the picture (see the left bottom corner or center bottom of 4b) and we loose some elements by thresholding (observe the disappearing of small circles in the upper left cornerr of 4a).

The final algorithm can be described as follows:

- Resize the picture (optionally).
- Use the Otsu algorithm for binarization of the picture
- Apply erosion filter with a circle–like structural element.
- Divide the set into connected components.
- Apply CEC in each cluster.
- Correct the radius of the circle obtained by CEC respectively to structural element which was used in erosion.



(a)



(b)

Fig. 4 The effect of the CEC algorithm

Our method works well in the case of resized pictures so fitting the parameters is quick. In general our method needs the following parameters:

- The level of thresholding (in this article we used the Otsu method).
- The size of a structural element in the erosion filter (we used approximately half of the radius of the smallest disks in a cluster)
- Two parameters requested by the CEC algorithm:
  - The starting number of clusters in each connected component (approximately the number of circles in the largest one)
  - The parameter describing the level of a minimal cluster size (we fixed it at 10% of the connected component size).

Fig. 4 presents the effect of our algorithm.

4 Conclusion

In this paper we present a new method of disc–like shapes detection in TEM pictures. As was mentioned earlier, in this situation we need to deal with elements which are not exactly disks, do not have smooth borders and in many cases they are not disjoint. Our approach, which is based on the CEC algorithm, allows us to deal with extracting this kind of elements.

The results of our investigation can be applied in the case of many types of nanomaterials with nanoparticles with spherical shapes. Moreover we can use the method to general disc detection in various type of images.

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