Measurement 92 (2016) 252–263

Contents lists available at ScienceDirect

Measurement

journal homepage: www.elsevier.com/locate/measurement

Quantifying shapes of nanoparticles using modified circularity and ellipticity measures

Lazar Kopanja [a,*], Dragiša Žunić [b], Boris Lončar [a], Sašo Gyergyek [c], Marin Tadić [d]

[a] Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, PO Box 3503, 11120 Belgrade, Serbia
[b] Faculty of Computer Sciences, John Naisbitt University, Bulevar umetnosti 29, 11070 Belgrade, Serbia
[c] Jožef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia
[d] Condensed Matter Physics Laboratory, Vinca Institute of Nuclear Science, University of Belgrade, POB 522, 11001 Belgrade, Serbia

ARTICLE INFO

Article history:
Received 31 January 2016
Received in revised form 30 May 2016
Accepted 11 June 2016
Available online 11 June 2016

Keywords:
Image analysis
Morphology
Particle shape
Particle characterization
Circularity
Elongation

ABSTRACT

We propose using a new circularity measure, and an ellipticity measure. Observing an example of hematite (α-Fe_2O_3) nanoparticles, we compared and discussed a new circularity measure, with a standard measure. It has been shown that using the new measure gives better results when working with low-quality images or with low-resolution images. Using the same images modified ellipticity measure has also been discussed. We have analyzed the problems arising from computing the elongation of a shape. We have shown that the standard approach to compute elongation is not appropriate for some particles. We presented the application of the modified approach to solve this problem.

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1. Introduction

New technologies and the development of materials, as well as the need for various new materials' properties, lead to development of new nanoparticle systems, in which it is possible to generate specific physical properties, which satisfy various requirements and needs in practical applications [1–8]. The relation between particle shape and its properties has been often studied in the literature [9–30]. Gholamrezaei et al. reported different morphologies of Ag_2Te nanostructures synthesized using $TeCl_4$ as a new precursor and hydrazine hydrate as reducing agent by a hydrothermal method [30]. They showed that important factor on degradation of dye in presence of photo-catalysts is the morphology of nanostructure [30]. Gholamrezaei et al. synthesized PbTe nanostructures via a simple solvothermal method with application of salen-Pb complex and salophen-Pb complex as precursors. The morphology of the products was affected by temperature [27]. The same authors prepared PbTe nanostructures via a hydrothermal reaction [28]. They presented the effects of different surfactants such as cationic, anionic, and polymeric surfactant on the morphology and purity of the products were investigated. Results showed that changing the capping agent can achieve different morphologies [28]. The efficiency and short circuit current (J_{SC}) value of solar cells are affected by the thin film's surface morphology and the morphology of $SrTiO_3$ nanostructures that were synthesized by modified sol–gel method [26]. Ahmed et al. synthesized CdS nanostructures of different shapes such as, nanoparticles (NPs), nanosheets (NS) and nanorods (NRs) one step chemical solvothermal method [31]. The effect of shape on optical and magnetic properties of CdS nanostructures was studied. The optical band gap and emission spectra are found to be shape dependent. CdS NRs were found to have high saturation (Ms) magnetization than that of CdS NPs and NS [31]. Shirato et al. presented that the aspect ratio of the particles is the most important factor that controls magnetic properties of various Co nanostructures (nanowires, nanorods and nanoparticles) [32]. Chakrabarty et al. prepared well crystalline α-Fe_2O_3 nanomaterials with a wide range of morphology variation by solvothermal route [Morphology dependent magnetic properties of α-Fe_2O_3 nanostructures [33]. They showed that the nanocoral shaped sample provides excellent magnetic moment at both 300 K and 5 K [33]. Zhou et al. synthesized spindle-like α-Fe_2O_3 structures via a hydrothermal method without using any hard templates or external magnetic field [34]. According to those results in the literature, spindle-like α-Fe_2O_3 exhibited relatively higher Ms. Zhang et al. reported a new

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[*] Corresponding author.

E-mail addresses: kopanjal@yahoo.com (L. Kopanja), dzunic@megatrend.edu.rs (D. Žunić), bloncar@tmf.bg.ac.rs (B. Lončar), saso.gyergyek@ijs.si (S. Gyergyek), marint@vinca.rs (M. Tadić).

http://dx.doi.org/10.1016/j.measurement.2016.06.021
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precursor-mediated growth of monodisperse magnetic cobalt ferrite ($CoFe_2O_4$) nanoparticles with controlled size and shape [35]. These $CoFe_2O_4$ nanoparticles exhibited different levels of peroxidase-like activities, in the order of spherical > near corner-grown cubic > starlike > near cubic > polyhedron [35]. Gupta et al. synthesized zinc oxide (ZnO) nanostructures of different morphology by simple soft-chemical approaches [36]. They found size, shape and defect concentration dependent ferromagnetic behavior and photocatalytic activity.

The increase of coercivity, along with increase of shape elongation of nanoparticle, has been discussed [37,38]. For example, increasing the elongation of iron (Fe) by factor 5, increase coercivity more than 10 times (from 820 to 10,100 Oe) [37]. It has been shown that, by varying the size and shape of nanoparticles in nanoparticle materials in wide spectrum, one can obtain the desired physical characteristics [19,39]. In general, coercivity increases with increased elongation, i.e., with the increase of anisotropy of a shape.

Image processing and image analysis is a multidisciplinary field, covering various aspects of mathematics, computer science, electronics and optics, and has important application in medicine, nuclear physics, information technology, astronomy, industry. Considering what has been said previously, it is important to have a method at hand, that clearly describes nanoparticles' shape, because shape descriptors are a powerful tool for this analysis [40–46]. Here we are discussing circularity, ellipticity and elongation of nanoparticles.

Simple equations for describing shapes have been studied in the literature, referring to particles whose shape range from a circle to a regular n-polygon [47,48]. Shape descriptors have been analyzed to determine how similar a given shape is to a square, rectangle, triangle [49,50] and several circularity measures have also been studied [46,51–57]. Bagheri et al. [55] have studied the correlation between circularity and sphereness of irregular shapes, and emphasized the importance of using more than one shape descriptor, having at hand various tools to measure the same shape. Existence of several shape measures referring to a same shape is important because no single descriptor is good enough to perform at high level in all situations [58]. Particle shape analysis of silica coated iron oxide (maghemite/magnetite) nanoparticle clusters (core–shell nanostructures with different thickness of the silica shell) was discussed using computational methods [59]. In this paper was introduced the "circularity coefficient" (k_{circ}) defined as the ratio of circularity measure $C_2(S)$ of nanoparticles core and circularity measure core–shell nanoparticles in order to answer the question how the shell affects the overall shape of the final core–shell structure, with respect to circularity. It was shown that the saturation magnetization strength can be easily adjusted by controlling the thickness of the silica shell [59].

In this article we present the new circularity measure, denoted $C_2(S)$, as a shape property which provides an answer to a question how circular is a given shape. This measure assigns the particle an intrinsic quantitative value, whilst in the same time, it is very simple to use. A circle is a shape that has a circularity measure 1 (1 stands for 100%). Besides, the measure we propose is invariant with respect to similarity transformations: translation, rotation, scaling. This is a very desirable property in applications. We will discuss the use of the new circularity measure, $C_2(S)$, and the standard measure, denoted $C_1(S)$, which, in Ref. [46] is denoted as R, and in Ref. [55] as φ_{Cox}.

Particles of elliptic shape are often considered in the literature [60,61]. In order to better describe particles, as a more general measure of circularity, we define an ellipticity measure, which determines how much a given shape differs from a perfect ellipse.

In order to apply this in tasks of classification, recognition, or identification of objects for every shape measure, it is expected i.e., a minimal requirement has to be invariant with respect to similarity transformations (translation, rotation, scaling).

2. Materials and methods

2.1. Synthesis

In a procedure for the synthesis of α-Fe_2O_3 nanoparticles, iron (0.2 M) solution was prepared in a beaker by mixing $Fe(NO_3)_2 \cdot 3H_2O$ (98%, Aldrich) in a distilled water. The above solution was mixed with urea (98%, Aldrich) or citric acid (98%, Aldrich) (0.1 M) under continuous stirring, and then it was transferred into Teflon-lined stainless steel autoclave of 80 mL capacity. The autoclave was maintained at 180 °C for 12 h and then cooled to the room temperature. The obtained red precipitates were washed several times with distilled water and ethanol to remove the impurities and then dried at 80 °C for 6 h. All chemicals used in our experiments are analytical reagents and used as received.

2.2. Circularity measures

Circularity, as one of the most standard shape descriptors, is often considered in the literature. Usually it is regarded as the ratio between shape's area and its perimeter [44–46,57,62,63]:

$$C_1(S) = \frac{4 \cdot \pi \cdot Area\_of\_S}{(Perimeter\_of\_S)^2}.$$

This circularity measure has several desirable properties as stated by the following theorem.

Theorem 1. *The circularity measure $C_1(S)$ satisfies:*

(a) $C_1(S) \in (0,1]$ *for all shape S,*
(b) $C_1(S) = 1 \Leftrightarrow S$ *is a circle,*
(c) $C_1(S)$ *is an invariant with respect to similarity transformations (translation, rotation, scaling).*

Circularity $C_1(S)$ depends on the area, but also on the perimeter of the shape considered. Calculating area is not difficult because it suffices to count the pixels contained within the shape [30], whilst computing the perimeter can be a harder task. Also, the image quality and change of resolution often influence the performance of $C_1(S)$ namely in case of changing brightness, or in the presence of narrow protrusions, there may be large differences between measured circularity. This is due to these effects increasing significantly the perimeter of a particle considered, which leads to a significant decrease of the value measured by $C_1(S)$.

Therefore, in order to avoid these drawbacks, we introduce the circularity measure based exclusively on an area of the shape considered, thus avoiding the computation of the perimeter.

Definition 1. When analyzing an arbitrary shape S whose centroid coincides with the origin, then the circularity $C_2(S)$ is defined as:

$$C_2(S) = \frac{1}{2\pi} \cdot \frac{Area(S)^2}{\min_{\theta \in (0,2\pi]} \iint_{S(\theta)} (x^2 + y^2)\,dxdy},$$

where $S(\theta)$ denotes the shape S rotated for θ around the origin, whilst $Area(S)$ represents an area of the shape considered, S.

The $C_2(S)$ measure has the desirable properties, the ones that we stated for $C_1(S)$. To derive the proof basic calculus is sufficient. The proof of (a) and (b) from Theorem 1 is based on the following equivalence:

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