



## A K-means Based Methodology for Evaluation of Shape Parameters for Nano-particles

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**Abstract**—In this work a new approach is proposed for determination of shape parameters of nano-particles using K-means and Mean shift algorithm. K-means is used to segment nano-particles in an image which are then processed to determine shape parameters. Here diameter, area, perimeter, aspect ratio, elongation, major axis, minor axis are calculated for TEM (Transmission Electron Microscopy) nano images. The method is successfully implemented on TEM images of Silver (Ag), Copper (Cu), and Gold (Au). A comparison is made between parameters calculated through proposed approach and manual approach. The methodology gives fast, accurate and robust results when compared with manual method. Statistical results are presented in the paper.

**Keywords**— Clusters, Seed-points, Nano-particles, Shape-parameters, Standard deviation.

### I. INTRODUCTION

Segmentation is an important aspect of image processing which finds its application in number of fields. K-means algorithm is used for cluster formation. [1] is Based on minimizing objective function. Given a set of n data points in space R, objective is to find k seed points in given space R so as to minimize mean square distance from seed point to center. It has various variants associated with it. It is a generalized form of Lloyds algorithm which was originally meant for scalar data.[2] puts it under the category of Squared error based clustering.[3] explains it in five steps as explained under :-

1. All objects are distributed randomly to K number of different clusters.
2. Mean value of each cluster is calculated and is used to represent the cluster.
3. Objects are redistributed to closest cluster according to distance from the cluster center.
4. Mean values are updated.
5. Criterion function E is calculated, until it converges.

$$E = \sum_{j=1}^k \sum_{i=0}^n \|x_i - m_j\|^2$$

Where E is total square error of all objects in data cluster.  $X_i$  is data object set,  $m_j$  is mean value of cluster  $C_i$ . [4] describes mean shift algorithm as feature space analysis. In this pixels having same set of convergence locations are given same segmentation levels. [5] defines a nanoparticles in two categories one fine particles whose diameter ranges between 100nm to 2500nm and ultra fine particles whose diameter ranges between 1nm to 100 nm. It is observed that each nanoparticle exhibit certain properties associated with it which differ significantly as compared when measured in bulk. Nanoparticles find various applications in almost every field of science such as targeted drug delivery, [6] Bio sensing, Bio imaging, [7] quantum computer, optical, electrical and magnetic devices. At nano level size and shape plays an important role. Once an image is obtained of nano-particle it is subjected for calculation of shape parameters by human eye. This approach is often tedious and chances of human error are more and also these are time consuming. It is open to human subjectivity as well. For this reason digital image processing is of much importance. [8] Explains the importance of various shape features. In this shape parameters of particles in images were calculated by means of linear contrast improving method and then applied histogram equalization on it.[9] Calculated various parameters and then graph were plotted. This work is carried out on images of nanoparticles which are taken using TEM of silver, copper, gold. A methodology is proposed which uses the concept of segmentation, contour-traversal, ellipse fitting to calculate shape parameters.

### II. PROPOSED METHODOLOGY

The proposed methodology is three phase process which are shown as following process flow.

In first phase mean shift is applied a prior to compensate the problem of finding accurate seed-points in K-means. Second phase takes segmented images as input and extracts contour which then is ellipse fitted. Third phase uses contour traversal for evaluating shape parameters.

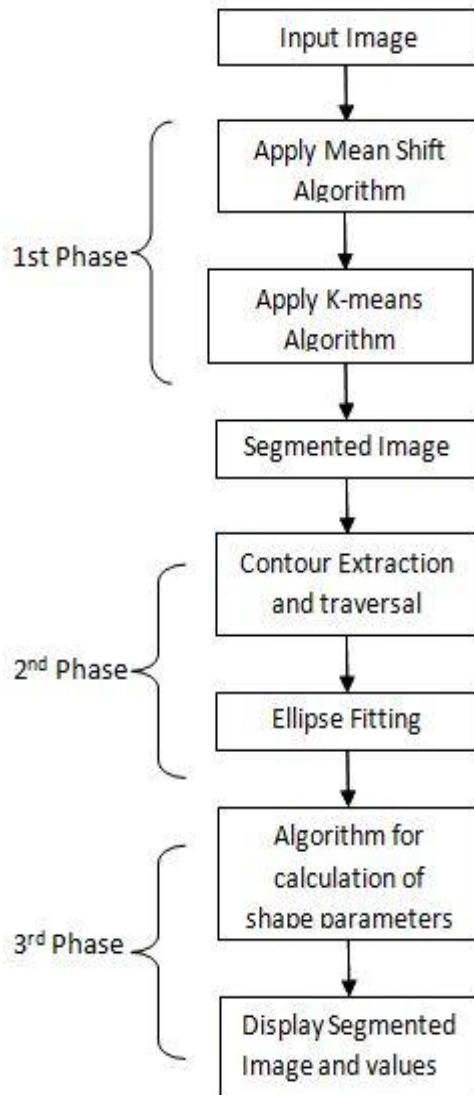


Fig. 1 Process flow of proposed method

### III. RESULT

Algorithm was applied on different images of gold, silver and copper .And results were calculated on 60 nano particles (20 particles in each image). Here in following table standard deviation (in nm) is represented for different shape parameters in both case i) by manual method using Axio-vision image analysis software by Carl Zeiss.ii) by proposed method.

TABLE 1  
STANDARD DEVIATION OF DIFFERENT PARAMETERS.

Parameter	Image1		Image2		Image3	
	Manual	Algorithm	Manual	Algorithm	Manual	Algorithm
Diameter	1.16660224	1.19504006	0.7252359	0.57088431	1.04765138	1.49931655
Area	19.5933545	19.871641	17.646088	12.5741536	17.0136058	21.7793944
Perimeter	3.665464	3.726947	2.278691	1.783361	3.291721	4.584999

Image on which results are calculated are as follows:-

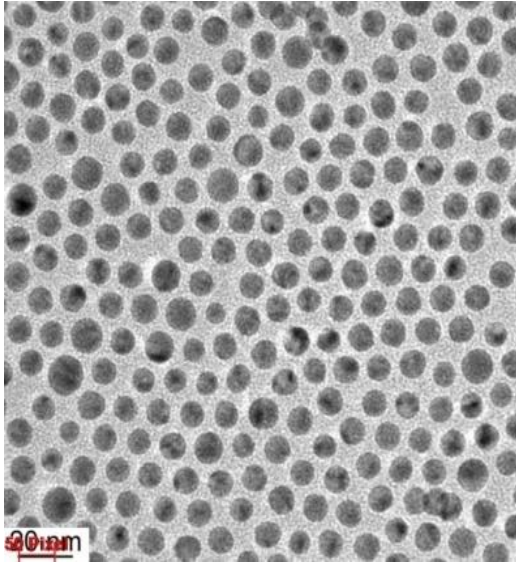


FIG 2 –IMAGE1

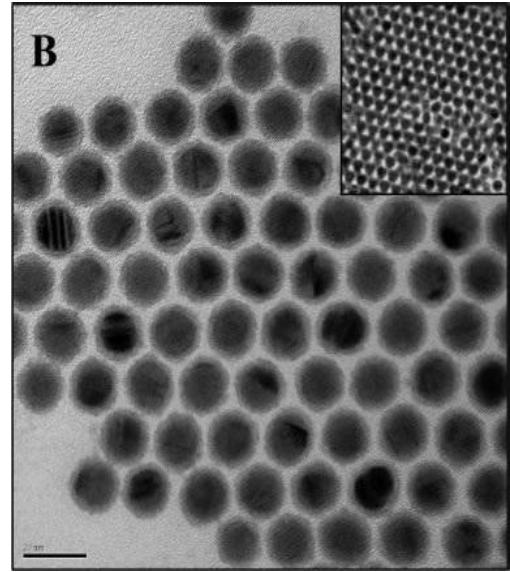


FIG 3 –IMAGE 2

Graphs are shown below for different images. For Image 1:-

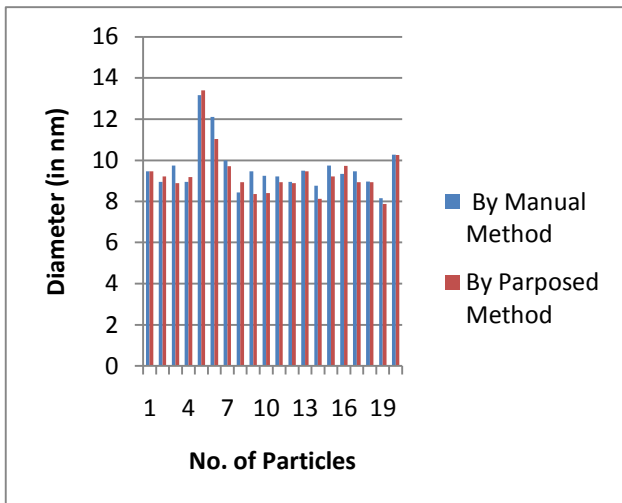


Fig 4-Diameter

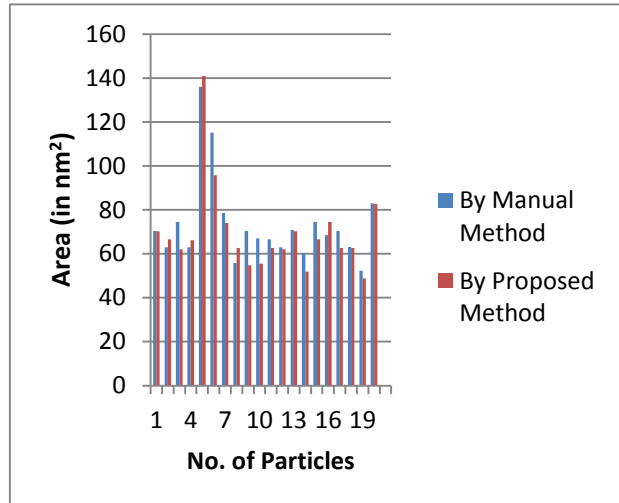


Fig 5-Area

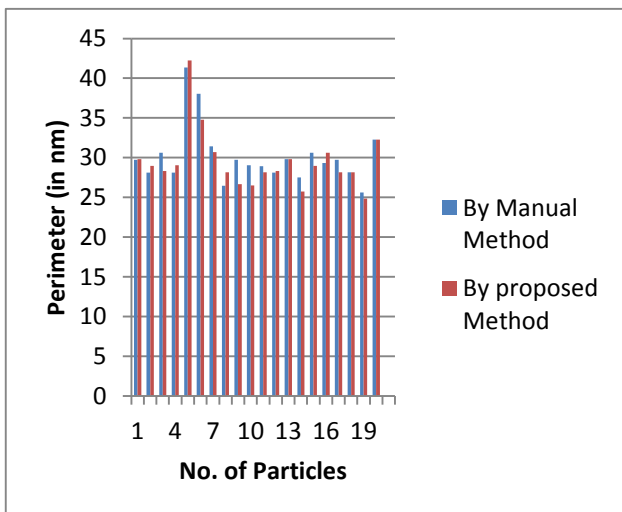


Fig 6-Perimeter

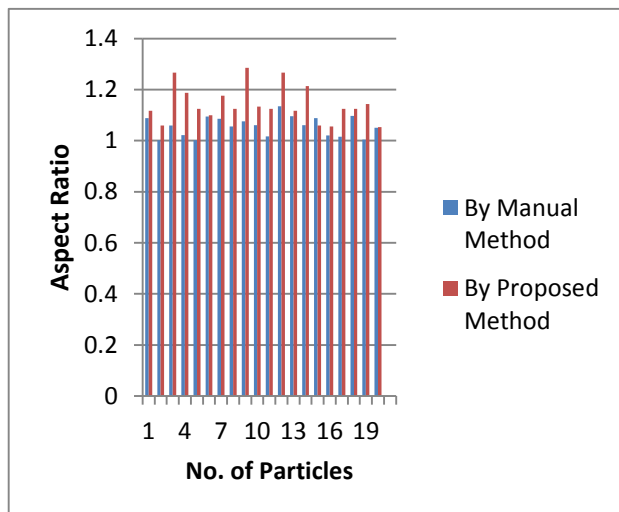


Fig 7-Aspect Ratio

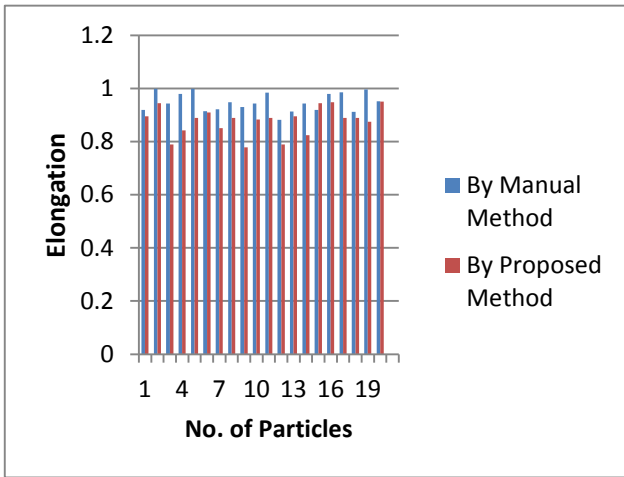


Fig 8 –Elongation

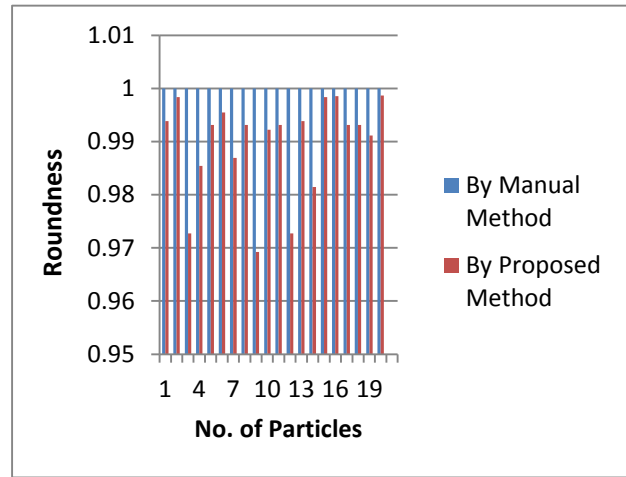


Fig 9-Roundness

For Image 2 Results are as follows:-

In image 2 size distribution of nanoparticles is uniform. So deviation from average value is less as variation in shape parameters of particles is less.

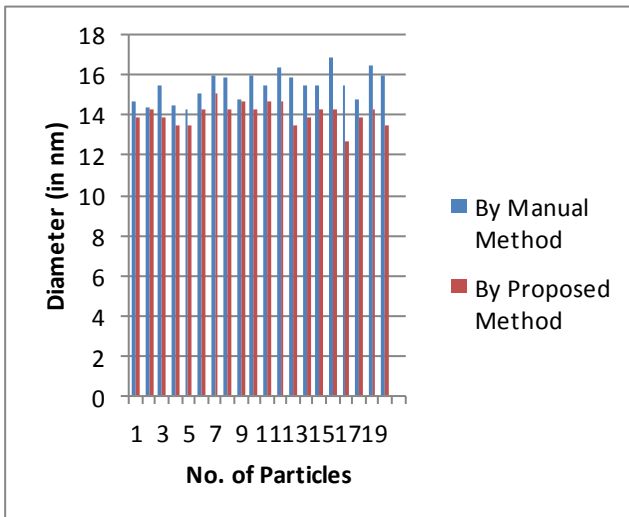


Fig 10-Diameter

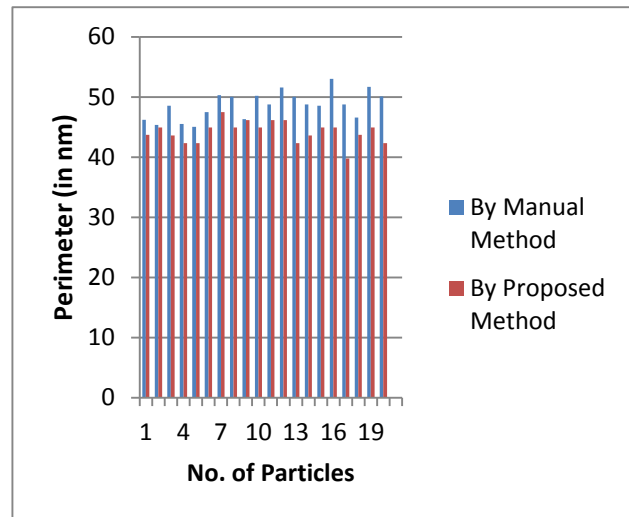


Fig 11-Perimeter

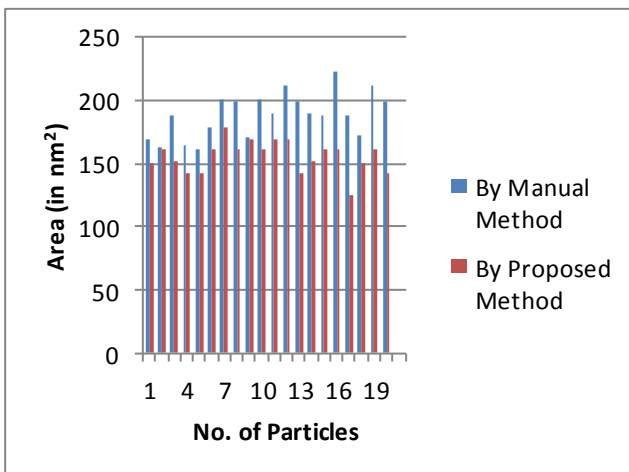


Fig 12-Area

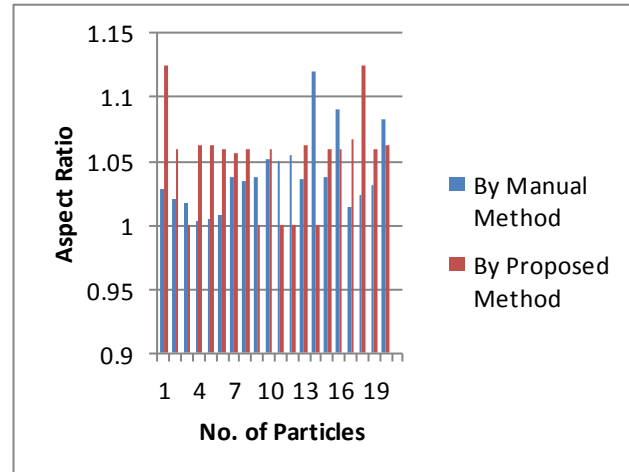


Fig 13-Aspect Ratio

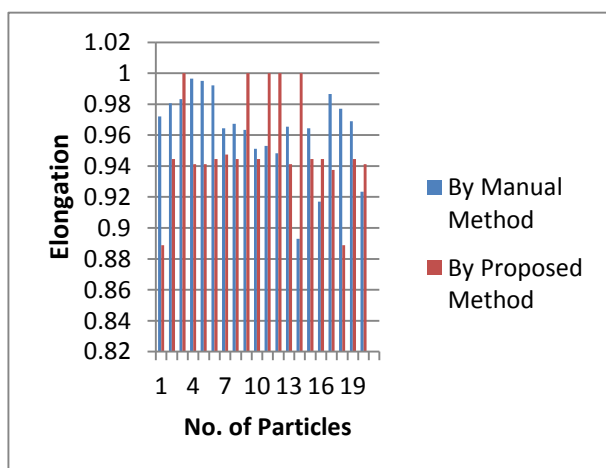


Fig 14 –Elongation

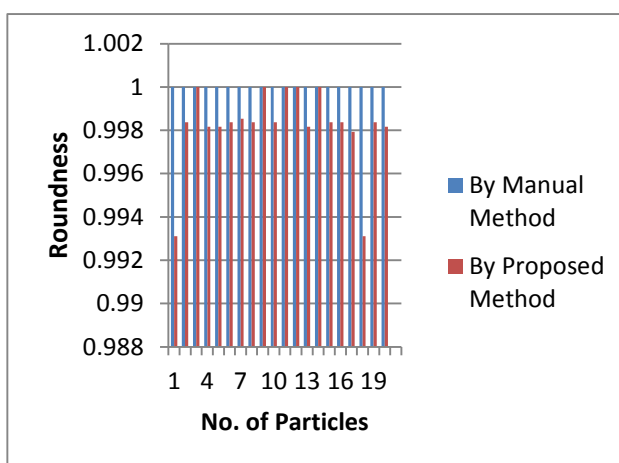


Fig 15-Roundness

#### IV. CONCLUSIONS

The Proposed methodology is implemented in OPENCV on 2.50GHz Intel Core i5 processor. Based on statistical data following conclusions are made:-

1. This method reduces the working time. For calculation of shape parameters of 20 particles manual approach take more than an hour, whereas in case of our proposed method calculation time is approximately 5-10 minutes for each image.
2. The method is more robust than the manual method. As in case of image 1 variation in size of nanoparticles is not uniform which is clearly indicated by standard deviation. For image 2 size of nanoparticles is comparatively uniform, which is well indicated by standard deviation.
3. Accuracy obtained is much higher and less error prone than manually.
4. As required modification and depending upon the domain, the methodology can be utilized for other fields i.e. like in metallurgy, bio science, in electrical and magnetic devices.

#### ACKNOWLEDGMENT

I will be failing in my duties if I do not express my sincere gratitude to Er. Harsimran Singh. It is because of their initiative, this work has been done.

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