JOURNAL OF DYNAMICS AND CONTROL

VOLUME 8 ISSUE 9

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BIOSYNTHESIZED MgO-ZnO METAL OXIDE NANOCOMPOSITE IMAGE ANALYSIS USING MACHINE LEARNING ALGORITHMS

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ABSTRACT: Metal oxide nanocomposites are the composites which are formed by combining two or more metal oxides. When two metal oxides, like MgO (Magnesium Oxide) and ZnO (Zinc Oxide), are combined, they will have improved stability, superior optical qualities, and increased catalytic activity. Different oxide components can interact to create synergistic effects that improve efficiency in applications such as sensors, photo catalysis, and antibacterial activity. This paper suggests biosynthesis of MgO-ZnO metal oxide nanocomposite using 5.12g of Mg $(NO_3)_2{\bullet}6H_2O$ (0.1M) (200mL) and 50ml rudanti fruit extract and using machine learning techniques for segmenting and classifying MgO-ZnO metal oxide nanocomposites based on their size and shape using machine learning approaches. We have used K-means segmentation and Random Forest classification machine learning techniques to extract the geometrical properties of these oxides. The size of each nanocomposite were extracted from the SEM image using the area of the pixels and categorized the segmented nanocomposites in various ranges such as: 0 nm–50 nm, 51 nm–100 nm, 101 nm–150 nm, 151 nm–200 nm, 200+ nm. The Random Forest classifier technique is used to categorize three different shapes namely circular, triangular, and elliptical. We have got 79% accuracy for classification of MgO-ZnO nanocomposites with f1-score (87%), precision (84%), and recall (91%).

KEYWORDS: Biosynthesized Metal Oxides, Image Analysis, MgO-ZnO, Nanocomposites, Machine Learning, K-means Clustering, Random Forest classifier.

1. Introduction

Nanocomposites, referred to as nanocomposites for essence, have shown widespread use in a range of industries. When two distinct oxides are combined to make multi oxide nanocomposites, the physical and chemical features of multimetal oxide nanocomposites such as band gaps, surface area and porosity, can be precisely controlled by adjusting the composition and production processes. This allows for the nanocomposites to be customized to fulfil specific application needs. Conventional analytical techniques, finds it difficult to analyze the size and shape of nanocomposites due to their tiny size and high surface area, to overcome these obstacles the machine learning techniques are applied. The MgO-ZnO nanocomposite SEM images which are synthesized using rudanti fruit extract are considered for this study. The original SEM image is preprocessed to remove noise and undesired artifacts to enhance image quality such as histogram equalization to enhance contrast, Gaussian blur to reduce noise, and edge enhancement. Afterwards the preprocessed image is segmented using K-means segmentation technique. Each segmented particle size is categorized into different size ranges based on their nanometer size. The segmented nanocomposites shape is categorized into three different shapes: circular, triangular, and elliptical. Finally, the accuracy of 79% with Random Forest classifier, with additional characteristics like F1-score, precision, and recall.

Determining the morphology of particle aggregates and agglomerates was developed by Théoden et al. [1]. Use of Artificial Intelligence algorithms to accurately and efficiently analyze and interpret SEM images of metallic nanocomposites was proposed by Gumbiowski , et al.[2]. automatic identification and delineating distinct regions or structures within Scanning Electron Microscopy (SEM) images of graphene to enhance the efficiency and accuracy of image analysis using U-Net neural network was suggested by Shah, Aagam, et al.[3]. Iron oxide nanoparticle size and shape analysis using machine learning algorithms has been proposed by Bannigidad, et al. [4]. Iron oxide nanocubes are being developed as a recognized reference material to provide precise and trustworthy calibration standards for nanocomposite size measurements were recommended by Abram et al. [5]. Microwave assisted green synthesis of MgO, Fe_3O_4 nanoparticles and Fe_3O_4–MgO nanocomposite using rudanti fruit extract was proposed by Gurubasavaraj, et al. [6]. The categorization of silver metal oxide nanoparticles based on the geometrical features such as size, shape was proposed by Bannigidad et al. [7]. The spatial arrangement of nanocomposites by fusing deep learning framework with centroid-to-contour distance measurements was suggested by Jang Jaeuk, and Hyunsoo Lee [8]. Deep learning-based particle size analysis using sophisticated algorithms to automatically and precisely identify particle sizes from images for improving efficiency and precision over conventional techniques presented by Kanchi et.al [9]. The use of machine learning algorithms for the analysis and interpretation of nanocomposite images by automating the size and shape characterization process was proposed by Glaubitz Christina, et al. [10]. A role of synthesis parameters on the shape and size of TiO_2

nanocomposites to analyze how variations in synthesis conditions affect the physical characteristics of TiO_2 nanocomposites was presented by Pellegrino, Francesco, et al. [11]. Applying machine learning algorithms to quantify and classify particle shapes, sizes, and distributions for enhancing precision and efficiency in material characterization has been developed by Lee et.al [12]. Machine learning techniques to predict the morphologies of nanocomposites based on their stability and growth conditions suggested by Yan, et al. [13]. Nanocomposite synthesis with machine learning algorithms to optimize and predict synthesis parameters has been proposed by Tao Huachen, et al. [14]. Use of machine learning algorithms, trained on labelled data to predict and analyse the 3D structures of metallic nanocomposites was proposed by Timoshenko Janis, et al. [15]. Use of machine learning algorithms to analyse and classify the shapes of convex nanocomposites in Transmission Electron Microscopy (TEM) images for precise measurement and characterization was developed by Wen, Haotian, et al. [16]. Manufacture of pure and mixed metal oxide nanocomposites and their antibacterial efficiency and cytotoxicity has been suggested by Stankic, et al. [17]. Developing accurate methods for producing uniform metal oxide and mixed oxide nanocrystals of controllable size and shape was developed by Nguyen, et al. [18]. Impact of geometrical features of nanocomposites on biological systems based on its interaction, uptake, dispersion, and toxicity was presented by Albanese Alexandre, et al. [19]. A simple and adaptable approach for producing magnetic oxide nanocrystals of chromium, manganese, iron, cobalt, and nickel with exact control over size and shape was suggested by Jana, Nikhil R., et al. [20]. Effect of size, shape, support, composition, and oxidation state of metal nanocomposites on their production and catalytic characteristics was proposed by Cuenya, Beatriz Roldan [21].

2 Materials and Methods

Biosynthesis of MgO-ZnO nanocomposite:

5.12g of Mg $(NO_3)_2{\bullet}6H_2O$ (0.1M) (200mL) and 50mL rudanti fruit extract were mixed in 500mL two necked flask. The mixture was stirred continuously at 85°C for 1hr. After that 5.94g of Zn $(NO_3)_2.6H_2O$ (0.1M) to above solution, after being cooled to room temperature the MgO-ZnO nanocomposites were collected by centrifugation (6000 rpm) and calcinated at 600°C for 5hr. The process of biosynthesis of MgO-ZnO nanocomposite is shown in fig.1.

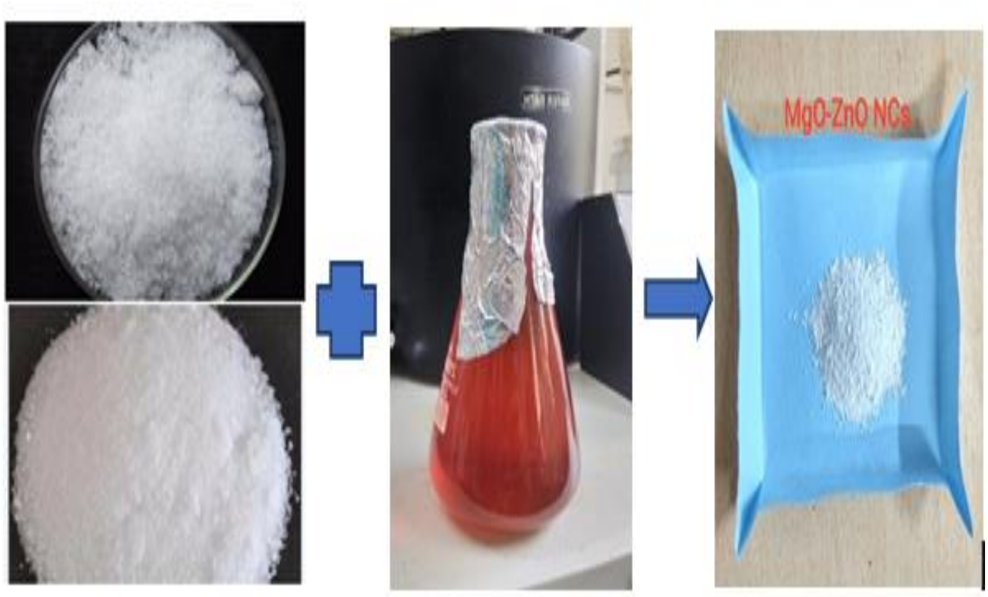


Fig. 1 Process of biosynthesis of MgO-ZnO nanocomposite

3 Proposed Method

The main objective of this study is to analyze the MgO-ZnO metal oxide SEM image biosynthesized at varying temperatures using 5.12g of Mg (NO3)2•6H2O (0.1M) (200mL) and 50mL rudanti fruit extract to study the geometrical features. The geometrical features of MgO-ZnO SEM image which are used in this study include; size, shape, major axis, minor axis, and diameter. These features are defined as follow:

- Size: Total number of pixels present in an extracted nanocomposite, which is given by
  Size =area_pixels*(scale_factor**2)
- Major Axis: Total number of pixels along the longest axis in a nanocomposite.
- Minor Axis: Total number of pixels along the smallest axis in a nanocomposite
- Diameter : The diameter of a nanocomposite is the distance across the particle, measured through the center.
  Diameter_nm= np.sqrt(4 * area_nm2 / np.pi)

The algorithm of this proposed study is as follow:

<u>Algorithm :</u>

Step 1: Input the original SEM image of MgO-ZnO.

Step 2: Apply CLAHE to enhance contrast and Gaussian blur to reduce noise.

Step 3: Apply morphological operations: Erosion and dilation to the preprocessed image.

Step 4: Apply K-means segmentation to the image with K=3 to segment the nanocomposites.

Step 5: Label the segmented nanocomposites.

Step 6: Calculate the size of each nanocomposite in nanometer scale.

Step 7: Determine the shape of each nanocomposite such as circular, elliptical, or triangular.

Step 8: Identification and classification of the nanocomposites based on their size and shape using Random Forest classifier.

Step 9: Store the detected nanocomposites as a knowledge base for further analysis and interpretation.

The flow diagram of the proposed methodology is given in the Fig.2

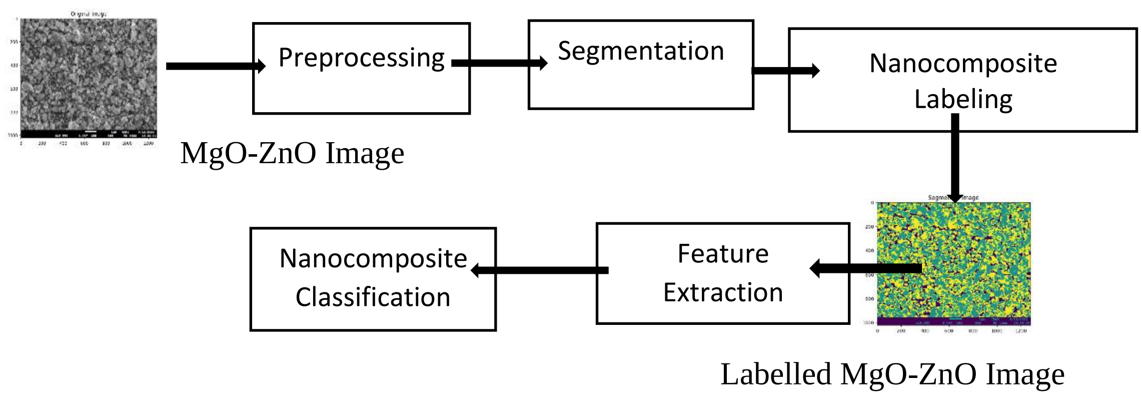


Fig.2: Flow diagram of the proposed methodology

3.1 Techniques for Classifying Nanocomposites Using Random Forest:

Random Forest is a versatile machine learning classification technique that can be quite effective for categorizing nanocomposites due to its ability to handle multimetal oxide nanocomposites and classify them based on their geometrical and shape properties. The number of collected nanocomposites is divided into train and test datasets using the Random Forest classifier. Working procedure of Random Forest classifier model is shown in Fig. 3.

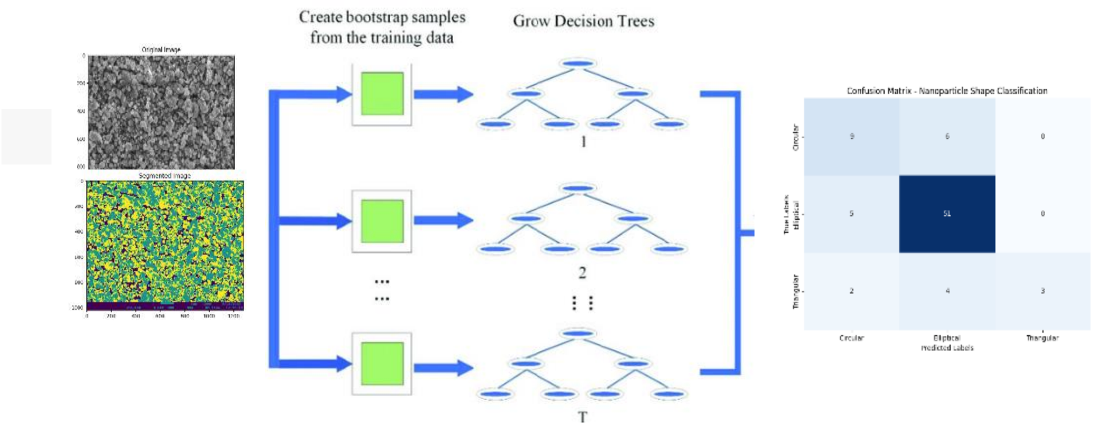


Fig. 3 : Working procedure of Random Forest classifier model

3.2 Performance metrics:

Accuracy, recall, precision, and F1-score are some of the common metrics that are normally used in order to assess the performance of machine learning models in image classification. These metrics are defined as follow:

a) Accuracy

The amount of accurate predictions made out of all the cases that were studied is known as accuracy, and it is calculated using the formula:

$$\textbf{Accuracy}=\frac{\mathbf{TP+TN}}{\mathbf{TP+TN+FP+FN}}$$

b) F1-Score

By calculating a weighted average of Precision and Recall, the F1-score provides a more sophisticated assessment of cases that are incorrectly classified. It uses this formula:

$$\textbf{F1-Score}=\frac{\mathbf{2*Precision*Recall}}{\mathbf{Precision+Recall}}$$

c)Recall

Recall, also known as sensitivity which represents the percentage of true positive cases among all actual positive cases. It is calculated using the formula:

$$\textbf{Recall} = \frac{\mathbf{TP}}{\mathbf{TP+FN}}$$

d) Precision

Precision is defined as the percentage of genuine positive instances among all anticipated positive cases. It is calculated using the formula:

$$\textbf{Precision} = \frac{\mathbf{TP}}{\mathbf{TP+FP}}$$

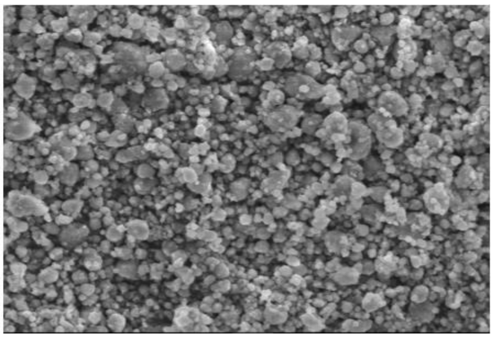
The confusion matrix, which is displayed in Fig. 5 displays the counts of False Positives, False Negatives, True Positives, and True Negatives. The terms like TP (True Positive), TN

(True Negative), FN (False Negative), and FP (False Positive) to denote the different combinations of expected and realized class outcomes in a test sample.

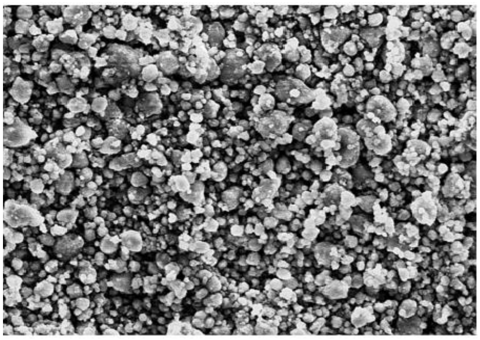
4 Experimental Results and Discussion

For the purpose of this experimentation, MgO-ZnO metal oxide nanocomposite SEM biosynthesized image is used. The preprocessing techniques are applied to reduce noise and to improve the image quality. The preprocessed image is then segmented using K-means segmentation technique. These results are displayed in Fig. 4. The segmented nanocomposites are labelled and size and shape of each nanocomposite is computed. Based on size, the nanocomposites are categorized into various ranges of [0 nm-50 nm], [51 nm-100 nm], [101 nm-150 nm], [151 nm-200 nm] and [200+ nm]. They are also categorized in different shapes namely circular, triangular and elliptical since these shapes are used to determine the applications of these metal oxide nanocomposites in various fields. The Random Forest classifier technique is used to classify the nanocomposites and achieved 79% accuracy for the classification.

Table 1 presents MgO-ZnO metal oxide nanocomposites with its size, range, and shape. A total of 829 nanocomposites are obtained from the MgO-ZnO SEM image. The Mgo-ZnO nanocomposites sizes are determined using the geometrical properties namely area, diameter etc. Table 2 shows categorization of Mgo-ZnO nanocomposites in different size ranges. The image processed and analyzed using Anaconda Jupyter notebook on an Intel(R) Core™ i5-10210U CPU@ 1.60 GHz.



(a)



(b)

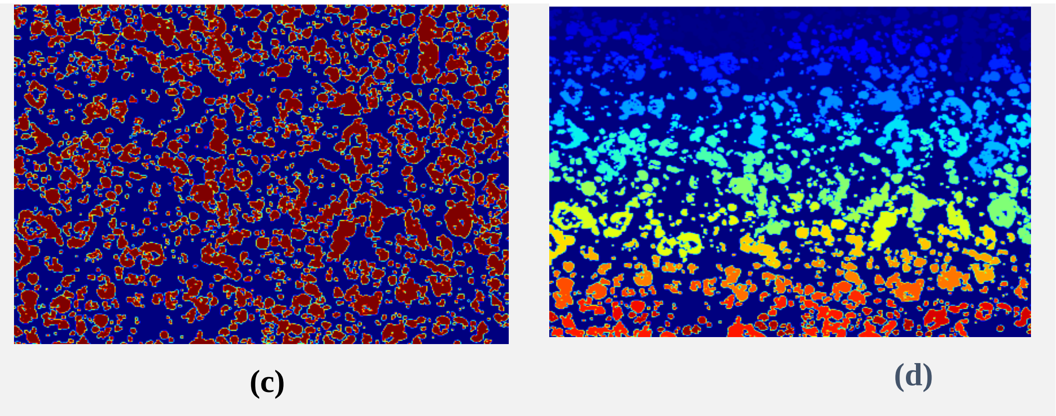


Fig. 4 a) SEM image of MgO-ZnO nanocomposite b) Preprocessed image c) Segmented image d) Labeled nanocomposite image

Table 1: MgO-ZnO metal oxide nanocomposites size, range, and shape

Composite No.	Size	Range	Shape
1.	6.38 nm	(0-50)nm	Triangular
2.	85.01 nm	(51-100)nm	Elliptical
3.	31.08 nm	(0-50)nm	Circular
4.	7.65 nm	(0-50)nm	Elliptical
…	…		
829.	11.81 nm	0-50	Elliptical

Table 2: Categorization of Mgo-ZnO nanocomposites in different size range

⬇Size Range/Shape ⟹	Circular	Triangular	Elliptical
(0-50)nm	91	4	231
(51-100) nm	77	2	190
(101-150) nm	27	1	84

(151-200) nm	12	0	38
200+nm	13	6	53
Total Nanocomposites	**220**	**13**	**596**

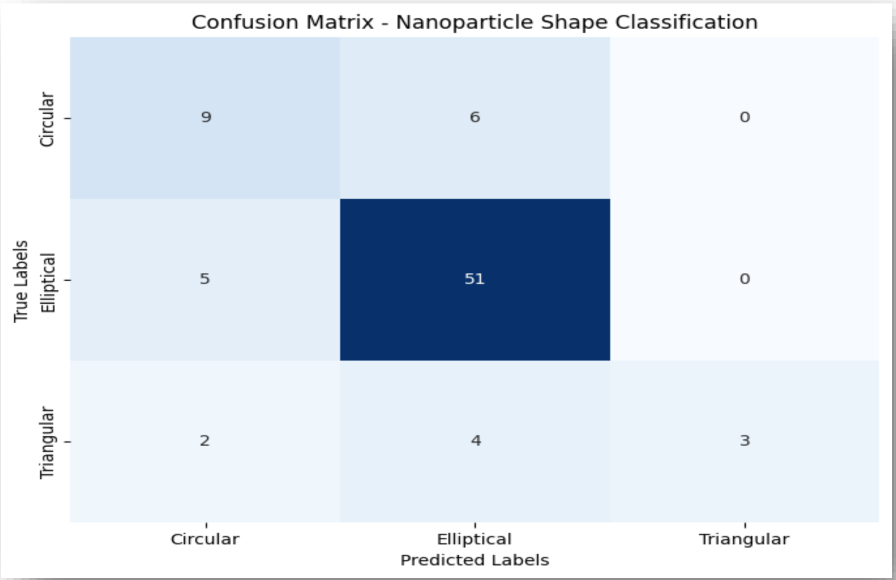


Fig. 5: Confusion Matrix for classifying total number of nanocomposites present in MgO-ZnO SEM image

It can classify the number of MgO-ZnO nanocomposites into three different shapes: circular, elliptical, and triangular. This experiment demonstrates that the majority of composites belong to the elliptical shape, while few composites belong to the triangular shape. The result of this technique is shown in Table 3.

Table 3: MgO-ZnO nanocomposites shape classification report using Random Forest technique

Shapes	No.of composites	Precision	Recall	F1-score	Support
Circular	16	0.56	0.60	0.58	15
Elliptical	61	**0.84**	**0.91**	**0.87**	56

Triangular	3	1.00	0.33	0.50	9
Accuracy				**0.79**	80
Macro Avg		0.80	0.61	0.65	80
Weighted Avg		0.80	0.79	0.78	80

5 Conclusion

The present study uses biosynthesized SEM images of MgO-ZnO multi metal oxide nanocomposites synthesized using rudanti fruit extract. This work is motivated by the fact that traditional characterization procedures are time-consuming and expensive. As a result, efforts are undertaken to automate a tool for determining the size of SEM images of MgO-ZnO multi metal oxide nanocomposites. This paper suggests segmenting and classifying MgO-ZnO multi metal oxide nanocomposites based on their size and shape using machine learning approaches. K-means technique is used to extract the size of each nanocomposites and categorized them in various ranges such as: 0 nm–50 nm, 51 nm–100 nm, 101 nm–150 nm, 151 nm–200 nm, 200+ nm. The Random Forest classifier technique is used to categorize three different shapes namely circular, triangular, and elliptical. We have got 79% accuracy for classification of MgO-ZnO nanocomposites with f1-score (87%), precision (84%), and recall (91%). The proposed results are analyzed and compared to manual results provided by chemical specialists, which show acceptable performance.

6 References

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