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Machine Learning for Characterization and Analysis of Microstructure and Spectral Data of Materials

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Abstract: In the contemporary world, there is lot of research going on in creating novel nano materials that are essential for many industries including electronic chips and storage devices in cloud to mention few. At the same time, there is emergence of usage of machine learning (ML) for solving problems in different industries such as manufacturing, physics and chemical engineering. ML has potential to solve many real world problems with its ability to learn in either supervised or unsupervised means. It is inferred from the state of the art that that it is essential to use ML methods for analysing imagery of nano materials so as to ascertain facts further towards characterization and analysis of microstructure and spectral data of materials. Towards this end, in this paper, we proposed a ML based methodology for STEM image analysis and spectral data analysis from STEM image of a nano material. We proposed an algorithm named Machine Learning for STEM Image Analysis (ML-SIA) for analysing STEM image of a nano material. We proposed another algorithm named Machine Learning for STEM Image Spectral Data Analysis (ML-SISDA) for analysing spectral data of STEM image of a nano material. We developed a prototype ML application to implement the algorithms and evaluate the proposed methodology. Experimental results revealed that the ML based approaches are useful for characterization of nano materials. Thus this research helps in taking this forward by triggering further work in the area of material analysis with artificial intelligence.

Subject Classification: *68U10*

Keywords: *Nano Material Characterization, STEM Analysis, Spectral Data Analysis, Machine Learning, Microstructure Analysis*

1. Introduction

With respect to growing research in nano materials and their characterization, there is increasing role of machine learning and artificial intelligence (AI). It is indispensable in the research of nano materials to understand and use AI based approaches for improving the designs and manufacturing of such materials. In this context, exploration of microstructures associated with nano-materials plays crucial role. At the same time ML based approaches are widely used to solve the problems in different domains. In manufacturing and many industries AI is being used for improving accuracy and quality in the designs. The role of ML is increasing in the study of new designs and implementation of nano materials [1].

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There are many existing methods that used ML approaches to leverage design and characterization of nano materials. In [4], [6], [7] and [8] machine learning models are used for characterization of complex materials. Chan et al. [4] focused on 3D sample characterization of autonomous microstructures with the help of machine learning. Holm et al. [6] studied the importance of machine learning for understanding and characterization of microstructures of materials. Xu et al. [7] explored machine learning and predictive modelling in order to have microscoping imaging. Their study helped in understanding microstructures pertaining Li-Ion batteries. Joshua et al. [8] considered complex materials in order to have data-driven machine learning to characterize surface microstructures. Infrared spectroscopy is used in their empirical study. There are certain studies where deep learning is used for studying materials. Lin et al. [3] investigated on the reconstruction and characterization of materials with the help of deep learning methods and their applications. Pokuri et al. [5] used a guided approach with interpretable deep learning for exploring microstructural properties associated with photovoltaics. Dimiduk et al. [13] explored different materials to ascertain the utility of ML and deep learning techniques. Their investigation caters to manufacturing innovation, material integration, processes, materials and structural engineering.

From the literature, it is inferred that it is essential to use ML methods for analysing imagery of nano materials so as to ascertain facts further towards characterization and analysis of microstructure and spectral data of materials. Our contributions in this paper are as follows. We proposed a ML based methodology for STEM image analysis and spectral data analysis from STEM image of a nano material. We proposed an algorithm named Machine Learning for STEM Image Analysis (ML-SIA) for analysing STEM image of a nano material. We proposed another algorithm named Machine Learning for STEM Image Spectral Data Analysis (ML-SISDA) for analysing spectral data of STEM image of a nano material. We developed a prototype ML application to implement the algorithms and evaluate the proposed methodology. The remainder of the paper is structured as follows. Section 2 reviews literature on methods of characterization and analysis of microstructure and spectral data of materials. Section 3 proposes a methodology for STEM image analysis and spectral data analysis from STEM image of a nano material. Section 4 presents results and discussion. Section 5 concludes on the results of the analysis and give scope for future work.

2. Related Work

This section reviews literature on different methods useful for material analysis. Dongdong et al. [1] focused on the process of characterization of coatings of thermal barrier with respect to microstructural features. They used a technology known as terahertz spectroscopy. Ramin et al. [2] focused on different techniques required for characterization of computational microstructures. Lin et al. [3] investigated on the reconstruction and characterization of materials with the help of deep learning methods and their applications. Chan et al. [4] focused on 3D sample characterization of autonomous microstructures with the help of machine learning. Pokuri et al. [5] used a guided approach with interpretable deep learning for exploring microstructural properties associated with photovoltaics. Holm et al. [6] studied the importance of machine learning for understanding and characterization of microstructures of materials. Xu et al. [7] explored machine learning and predictive modelling in order to have microscoping imaging. Their study helped in understanding microstructures pertaining Li-Ion batteries. Joshua et al. [8] considered complex materials in order to have data-driven machine learning to characterize surface microstructures. Infrared spectroscopy is used in their empirical study. Iquebal et al. [9] investigated on lithography process that is nanoindentation based. Their study is on acoustic emission signatures. Their empirical study was for characterization of rapid microstructures. Chowdhury et al. [10] used ML with images in order to understand and reconstruction of microstructures.

Du et al. [11] explored ML along with robotics for understanding the potential of materials pertaining to OPV. Pilania [12] used ML for different purposes that range from predictions of characteristics to autonomous design of materials. Dimiduk et al. [13] explored different materials to ascertain the utility of ML and deep learning techniques. Their investigation caters to manufacturing innovation, material integration, processes, materials and structural engineering. Ren et al. [14] proposed a protocol for vibrational spectroscopy with machine learning for understanding spectrum based structure and spectrum prediction. DeCost et al. [15] focused on the characterization of AM powder with the help of ML and computer vision. Konstantopoulos et al. [16] performed different kinds of testing on properties of materials for microstructure identification using ML approaches. Ruoqian et al. [17] focused on the composite microstructures that are of three-dimensional in nature. They used machine learning models that are context aware and the modelling of elastic localization is carried out.

Akshay et al. [18] explored computational materials in order to understand microstructures and they used spectral density function for empirical observations. Ruoqian et al. [19] proposed methodology using ML approaches for possible materials design and microstructure optimization. Xu et al. [20] proposed a design and representation approach based on ML for making microstructures with heterogeneity. Chen et al. [21] explored photoacoustic spectroscopy through machine learning for prostate cancer identification. From the literature, it is inferred that it is essential to use ML methods for analysing imagery of nano materials so as to ascertain facts further towards characterization and analysis of microstructure and spectral data of materials.

3. Methodology

We proposed a methodology based on methods of machine learning for analysing STEM images and spectral data of such materials. It is understood that ML plays crucial for understanding materials and characterization. STEM image of nano material is subjected to two kinds of procedures for characterization of material. This kind of study paves way for manufacturing novel nano materials and understanding the spectral data of materials. The given STEM image is subjected to ML based methods for analysis. The input is also subjected to spectral data analysis through decomposition in order to characterize materials. Figure 1 shows an overview of the proposed methodology for characterization of materials through ML methods.

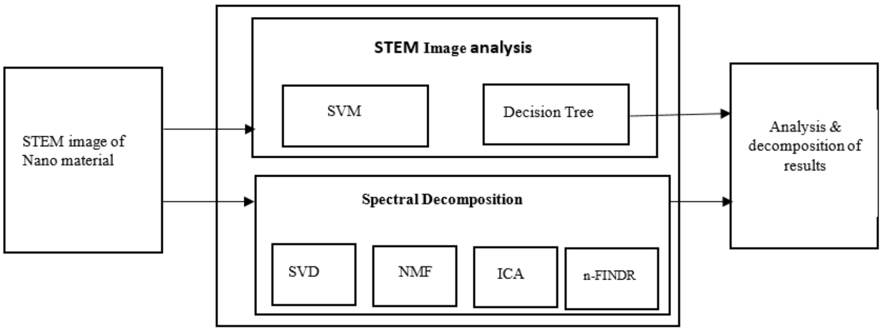


Fig 1: Overview of the proposed methodology used for STEM image analysis and spectral decomposition

The given STEM image is subjected to STEM image analysis with the help of ML models such as Support Vector Machine (SVM) and Decision Tree (DT). Afterwards, the spectral data analysis is carried out using Singular Value Decomposition (SVD), n-FINDR, Independent Component Analysis (ICA) and non-negative matrix factorization (NMF). SVM is one of the widely used ML classifier used for the study of materials. SVM is the binary classification algorithm which can divide the feature space into two classes based on its hyperplane criteria. Hyperplane approach can be expressed as in Eq. 1.

$$H{:}w^T(x) + b = 0 \quad (1)$$

The modus operandi of the SVM also needs a distance measure that is useful in determining classes in the process of STEM image analysis. The distance measure is expressed in Eq. 2.

$$D=\frac{|ax_0+by_0+c|}{\sqrt{a^2+b^2}} \quad (2)$$

There is also need for finding distance from given point to hyperplane equation in order to make the decisions while analysing STEM images. This distance computation is carried out as in Eq. 3.

$$d_h(\emptyset(x_0))=\frac{|w^T(\emptyset(x_0))+b|}{||w||_2} \quad (3)$$

Apart from SVM, DT is another important classifier used to analyse STEM image of a nano material. The decision tree classifier is based on identification of attribute or feature for splitting data while making decision tree. It is based on two measures known as entropy and gain as expressed in Eq. 4 and Eq. 5.

$$\text{Entropy(S)}=\sum_{i=1}^{c} -p_i log_2 p_i \quad (4)$$

$$\text{Gain(S, A)= Entropy(S)- } \sum_{\vartheta \epsilon Values(A)} \frac{|S_\vartheta|}{|S|} \text{ Entropy}(S_\vartheta)$$
(5)

Both entropy and gain measures are used for making decisions while modelling data using DT classifier. With respect to spectral data analysis, the given STEM image is subjected to spectral decomposition that is carried out using different methods such as Singular Value Decomposition (SVD), n-FINDR, Independent Component Analysis (ICA) and non-negative matrix factorization (NMF). The Singular Value Decomposition (SVD) is one of the methods used for analysing given material. SVD of a matrix is nothing but factorization of different matrices. It is used to explore linear transformations with theoretical and geometrical insights. In the domain of data science SVD has important applications due to its intuition in acquiring geometrical meaning. The SVD analysis can be expressed as in Eq. 6.

$$C_{m\times n} = U_{m\times r} \times \sum_{r\times r}. \times V^1_{r\times n} \quad (6)$$

Non-Negative Matrix Factorization is another technique used for decomposition of materials. For a given matrix NMF considers only non-negative elements. Considering W and H are two matrices, and A is original input matrix, the process of NMF is expressed as in Eq. 6.

$$A_{m\times n} = W_{m\times k}H_{k\times n} \quad (7)$$

Independent Component Analysis (ICA) is another ML technique widely used for separating different independent sources available in a given mixed signal. It focuses on independent components unlike principal component analysis. Considering there are different sources, ICA is computed as in Eq. 8.

$$[X_1, X_2, \ldots \ldots, X_n] \Rightarrow [Y_1, Y_2, \ldots \ldots, Y_n] \quad (8)$$

Another method of ML known as n-FINDR is used for spectral data analysis. It is widely used method for discovering endmembers from hyperspectral imagery. It exploits all p-endmember combinations in order to arrive at the desired results.

Algorithm Design

We proposed an algorithm named Machine Learning for STEM Image Analysis (ML-SIA) for analysing STEM image of a nano material. We proposed another algorithm named Machine Learning for STEM Image Spectral Data Analysis (ML-SISDA) for analysing spectral data of STEM image of a nano material. We developed a prototype ML application to implement the algorithms and evaluate the proposed methodology.

Algorithm: STEM Image Analysis (ML-SIA)

Inputs:

STEM image of an oxide catalyst ***I***

Machine learning classifier pipeline ***P***

(P refers to a collection of classifiers consisting of SVM and DT)

Training data ***T***

Output:

Results of STEM image analysis ***R***

1. Start
2. F←ExtractFeatures(***I***)
3. For each ML technique t in P
4. model←TrainClassifier(T)
5. ***R***←FitModel(M,F, I)
6. Display ***R***
7. End For
8. End

Algorithm 1: STEM Image Analysis (ML-SIA)

As presented in Algorithm 1, the given input STEM image is subjected to classification using different ML models such as SVM and DT. The pipeline of these models, training data T and STEM image of an oxide catalyst are inputs to the algorithm. It has an iterative process in order to perform STEM image analysis and provide results. Machine Learning for STEM Image Spectral Data Analysis (ML-SISDA) is another algorithm proposed.

Algorithm: Machine Learning for STEM Image Spectral Data Analysis (ML-SISDA)
Inputs:
STEM image of an oxide catalyst ***I***
Machine learning models pipeline ***P***
(P refers to a collection of ML models such as Singular Value Decomposition (SVD), n-FINDR, Independent Component Analysis (ICA) and non-negative matrix factorization (NMF))
Output:
Results of STEM image spectral data analysis ***R***

1. Start
2. Spectral←Extract(***I***)
3. For each ML model m in P
4. r←SpetralDataAnalysis(spectral)
5. Add r to ***R***
6. End For
7. Display R
8. End

Algorithm 2: Machine Learning for STEM Image Spectral Data Analysis (ML-SISDA)

As presented in Algorithm 2, it takes STEM image of an oxide catalyst and machine learning models pipeline as input and returns the results of STEM image spectral data analysis. It extracts spectral features of given input image. Then it has an iterative process to analyse spectral data in different aspects and generate visual representations of spectral data for characterization of nano materials. This is the ML approach that has potential to improve the state of the art.

4. Results and Discussion

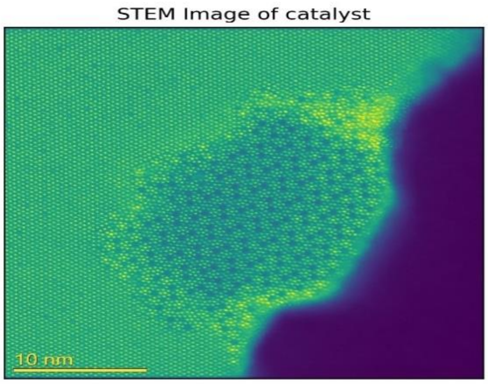
This section presents experimental results of the proposed methodology that covers STEM image analysis and spectral data analysis from STEM image of a nano material. The proposed algorithms are evaluated with an input image which is nothing but a STEM image captured from a nano material pertaining to an oxide catalyst. Different ML techniques are used for the empirical study. They include SVM, DT, SVD, NMF, ICA and n-FINDR.

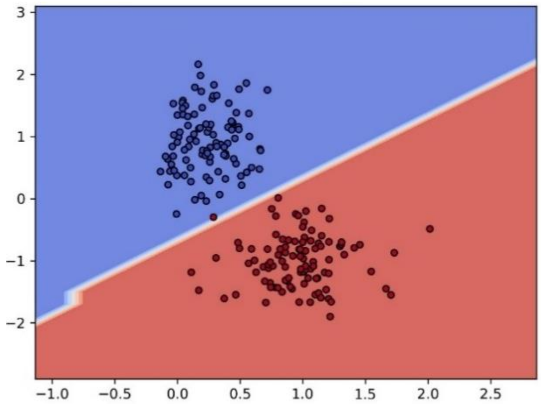
The results are divided into the results of STEM image analysis and STEM spectral data analysis.

4.1 Results STEM Image Analysis

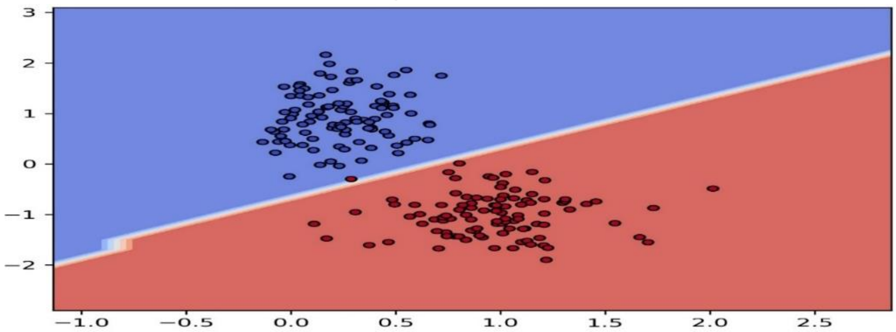
Two popular ML algorithms known as SVM and DT are used to characterize and analyse a STEM image captured from a nano material pertaining to an oxide catalyst. The two classification models do have different modus operand in analysing and coming up with required classes. Two classes are used for the analysis.

As presented in Figure 2 (a), it reflects a STEM image of an oxide catalyst. Scanning transmission electron microscopy imaging technology is used to know the characteristics of nano materials. Figure 2 (b) the result of SVM classification of STEM image is provided. It is binary classification that has resulted in two classes based on SVM's approach in hyperplane for classification. Figure 2 (c) shows classification result performed by Decision Tree algorithm with two classes. This classification is based on the ability of DT algorithm in identifying attribute for splitting.





(a) Input STEM image **(b) Result of analysis with SVM**



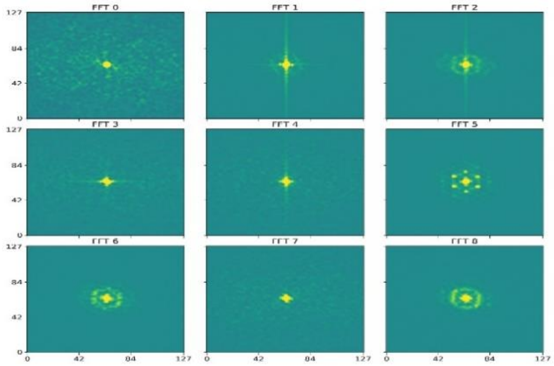
(c) Result of analysis with DT

Fig 2: STEM image analysis

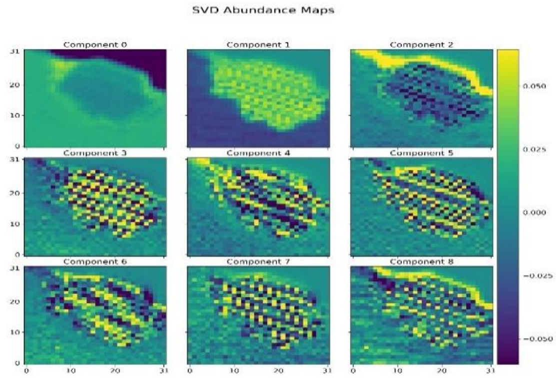
4.2 Results Spectral Data Analysis

Different methods are used for spectral data analysis provided a STEM image as input. The methods used for the empirical study are SVD, NMF, ICA and n-FINDR.

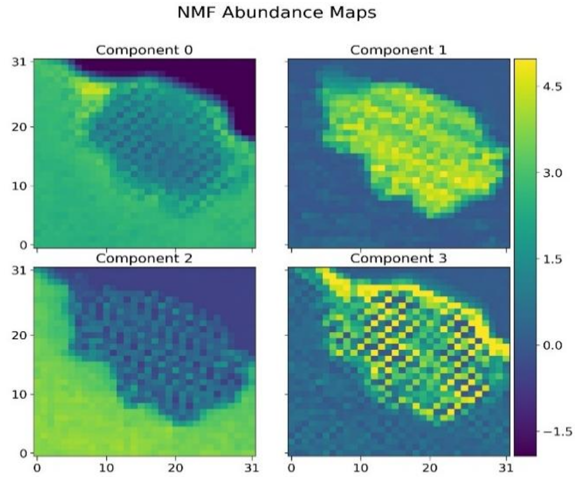
Figure 3 (a) shows FFT windows are used based on sliding window approach for performing spectral data analysis. Figure 3 (b) shows SVD abundance maps in order to analyse spectral data. It shows different components reflecting visualization of SVD abundance maps that are used to ascertain the spectral data associated with given STEM. Figure 3 (c) shows NMF abundance maps are visualized with the help of NMF coefficients. Figure 3 (d) shows that NMF components are used to visualize then and it can be used for effective spectral data analysis.



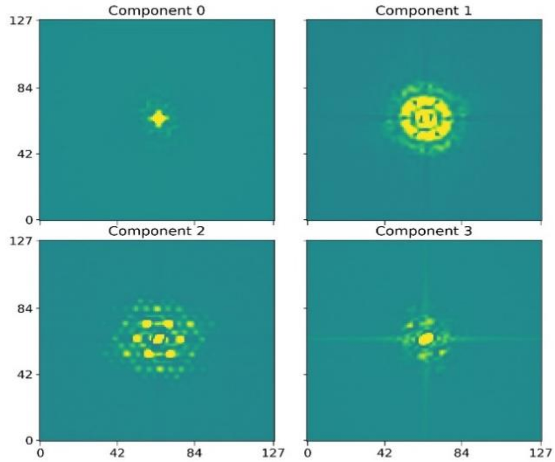
(a) Spectral data analysis in terms of FET



(b) **Spectral data analysis in terms of SVD abundance maps**



(c) Spectral data analysis in terms of NMF abundance maps



(d) **Spectral data analysis in terms of components**

Fig 3: Spectral data analysis

5. Conclusion and Future Work

In this paper, we proposed a ML based methodology for STEM image analysis and spectral data analysis from STEM image of a nano material. We proposed an algorithm named Machine Learning for STEM Image Analysis (ML-SIA) for analysing STEM image of a nano material. We proposed another algorithm named Machine Learning for STEM Image Spectral Data Analysis (ML-SISDA) for analysing spectral data of STEM image of a nano material. We developed a prototype ML application to implement the algorithms and evaluate the proposed methodology. Experimental results revealed that the ML based approaches are useful for characterization of nano materials. Thus this research helps in taking this forward by triggering further work in the area of material analysis with artificial intelligence. In future, we intend to explore deep learning models for nano material analysis for improving the benefits of characterization of nano materials. This will help in many industries such as manufacturing of storage devices to improve quality and productivity.

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