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Intelligent Material Characterization: A ML Approach for Predicting Microstructure of Nanomaterials

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ABSTRACT

Nanomaterials are important for many businesses today, such as computer chips and cloud storage devices. A lot of study is being done to make new nanomaterials at the same time, machine learning (ML) is being used more to solve problems in fields like physics, chemical engineering, and manufacturing sector. Because ML is capable of developing in both controlled and unstructured ways, it could help solve many problems in the real world. Using ML techniques for examining at images of nanomaterials is necessary to find out more about them and characterize and analyze their architecture and spectral data, according to the current state of the art. In order to achieve this, researchers presented in this study a ML based approach for analyzing Scanning transmission electron microscopy (STEM) images and spectral data from STEM images of nanomaterials. To analyze STEM images of a nanomaterial, researchers suggested an approach called Machine Learning for STEM Image Analysis (ML-SIA). In order to analyze the spectrum data of a STEM image of a nanomaterial, researchers have introduced an approach called ML for STEM Image spectrum Data Analysis (ML-SISDA). To execute the algorithms into practice and assess the suggested methods, researchers created a prototype ML application. According to experimental findings, ML-based methods are effective for characterizing nanomaterials. Therefore, by spurring more research in the field of material analysis using AI, this research assists in moving this into the future.

1. Introduction

The use of Machine learning as well as artificial intelligence are becoming more and more important in the expanding field of nanomaterials research and characterization [1]. Understanding and using AI-based techniques to enhance the designs and production of nanomaterials is essential to their development. Microstructures of nanomaterials are in need of to be studied more in this situation [2-4]. To solve problems in many different areas, ML-based methods are also used extensively. Deep learning is used to make ideas more accurate and high-quality in many fields, including manufacturing [5]. In the research of novel technologies and the use of nanomaterials, ML is becoming more important.

The importance of predictive modelling in the study of nanomaterials is also immense. Researchers can model how materials behave in different situations by using machine learning methods like CNNs as well as RNNs [6-10]. This helps them find new materials with special qualities. This ability to predict the future is especially useful for making nanoparticles better for specific uses, like electrical and biological devices, energy storage, and technology [11]. Additionally, combining machine learning with spectroscopy methods like IR as well as terahertz spectroscopy has made it easier to analyze spectral data more accurately, which has led to a better understanding of how materials are put together and how they interact with each other [13-16].

Leveraging ML techniques to improve nanomaterial design and characterization is an established practice. Complex materials are characterized using ML algorithms. [6-9] focuses on using ML for three-dimensional sample characterization of autonomous microstructures. [17-19] looked at how ML may help with material microstructure comprehension and characterization. [20-22] investigated microscoping images via the use of ML and predictive modeling. Their research contributed to the knowledge of Li-Ion battery microstructures. to analyze surface microstructures using data-driven ML, complicated materials must be addressed. They conducted their empirical investigation using infrared (IR) spectroscopy. It is used for certain assignments to find study tools that use DL. The study [23] looked into how DL methods can be used to recreate and characterize materials and what their applications. When [24] examined into the microstructural features of photovoltaics, they used a directed method with interpretable DL. ML along with DL methods have been examined in different sources to determine how useful they're actually [25]. Their research focuses on structural engineering, processes, materials, innovation in manufacturing, and material integration.

The research suggests that in order to determine facts for further characterization and evaluation of materials' microstructure and spectrum data, ML techniques must be used to analyze images of nanomaterials. The following are the contributions researcher made to this article. For the analysis of STEM images and spectral data from STEM images of a nanomaterial, researchers suggested an ML-based technique. For the analysis of STEM images of nanomaterials, researchers suggested an approach called ML-SIA. To analyze the spectrum data of a STEM image of a nanomaterial, researcher suggested a different approach called ML-SISDA. To test the suggested methods and put the algorithms into practice, researchers created a prototype ML application. The next section of the article is organized in the following way. Methods for analyzing spectral data and STEM images of nanomaterials are presented in Section 2. Findings and analysis are brought forth in Section 3. Finally, Section 4 provides some conclusions and areas for further research based on the study.

2. Methodology

The suggested technique utilizes ML to analyze STEM pictures and spectral data. ML is well known to be rather important for material understanding and characterization. Characterization of material using two types of processes with STEM images of nano materials. This kind of research opens the door for producing unique nano materials and knowledge of the spectrum data of materials. Analysis of the provided STEM picture is done using ML based approaches. To identify materials, the input is additionally decomposed and through spectral data analysis.

The general outline of the suggested approach for characterizing materials using ML approaches is shown in Figure 1.

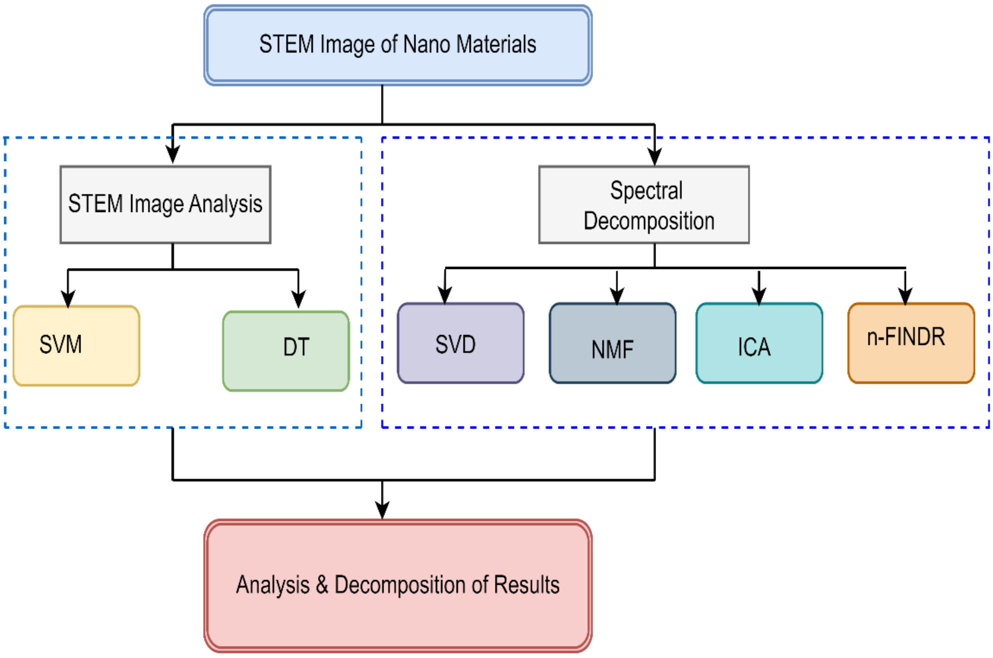

Figure 1 Schematic View of Proposed Methodology.

The provided STEM image is analyzed using ML models like Decision Tree (DT) and Support Vector Machine (SVM). Following that, non-negative matrix factorization (NMF), Independent Component Analysis (ICA), n-FINDR & Singular Value Decomposition (SVD) are used to analyze the spectral data. One of the popular ML classifiers for material analysis is SVM. Based on its hyperplane criterion, the binary classification method SVM may split the feature space to two groups. The hyperplane method may be written as seen in Equation 1.

$$\sum_{i=1}^{n} w_i\, x_i + b = 0 \qquad (1)$$

Where w_i indicates the component of vector weight w, x_i represents the component of point x, and b indicates the bias.

In order to determine classes throughout the STEM image analysis process, the SVM's method of operation also requires a distance measure. The distance measurement is provided in Eq. 2.

$$D = \frac{|w^T X_0 + b|}{||w||} \qquad (2)$$

Here, W = [a,b] indicates the normal vector to the line.

$x_0 = (x_0, y_0)$ represents the given point.

$w^T x_0$ indicates the dot product of the normal vector and the point.

$||w|| = a^2+b^2$ is the magnitude (norm) of the normal vector.

The absolute value ensures the distance is always positive.

Finding the distance from a given point to a hyperplane equation is also necessary for making choices about STEM pictures. This distance calculation is done according to Eq. 3.

$$D = \frac{|w^T x' + b|}{\|w\|_2} \qquad (3)$$

Here $x'=\phi * x_0$ indicates the feature transformation of x_0 into a HD space, $w^T x'$ represents the dot product between weight vector w and transformed point and $\|w\|_2 = \sqrt{\sum w_i^2}$ signifies the L2 norm of w, ensuring scale invariance.

DT is a significant indicator that is also used for examining at STEM images of nanomaterials. When making a decision tree, the DT algorithm uses a characteristic or feature to divide the data into groups. The two measurements that it uses are entropy and gain, which are shown in Equations 4 and 5.

$$H(S) = -\sum_{i=1}^{c} p_i \, log_2 p_i \qquad (4)$$

Here H(S) is used to measures the uncertainty in dataset S, c indicates the Number of possible classes, p_i represents the likelihood of class occurrence i at the dataset, $log_2 p_i$ represents the quantity of data acquired whenever an event happens with a likelihood of p_i, the negative sign guarantees that entropy remains non-negative.

$$IG(S, A) = H(S) - \sum_{v \epsilon values(A)} \frac{|S_v|}{S} H(S_v) \qquad (5)$$

When employing a DT classifier to model data, assessments are made utilizing both the entropy and gain measurements. Employing a variety of techniques, like SVD, n-FINDR, ICA, and NMF, the provided STEM picture is subjected to spectrum decomposition with respect to spectral data analysis. One tool used for material analysis is the SVD. Factorization of several matrices is all that the SVD for a matrix. Leveraging theoretical and geometrical understanding, it is used to investigate linear transformations. SVD's intuitive ability to comprehend geometric meaning makes it a valuable tool in the data science field. Equation 6 may be used to represent the SVD analysis.

$$C_{m\times n} = U_{m\times r} * \Sigma_{r\times r} * V_{r\times n}^T \qquad (6)$$

Here $C_{m\times n}$ indicates the original matrix, $U_{m\times r}$ represents the orthogonal matrix, $\Sigma_{r\times r}$ signifies the diagonal matrix, and $V_{r\times n}^T$ indicates the transpose of an orthogonal matrix.

Non-negative matrix Material breakdown can also be done through factorization. Considering a certain matrix, NMF solely looks at elements that are not negative. Equation 7 shows the NMF process, where W as well as H are 2 matrices & A is the original input matrix.

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

Another popular ML method for identifying the several independent sources present in a given mixed signal is ICA. In contrast to principal component analysis, it concentrates on independent elements. Considering into account the various sources, ICA is calculated using Equation 8.

$$Y = f(X) \quad (8)$$

Where f represents the function applied to input X for acquiring the output Y, $X\ takes\ the\ value\ from\ X_1 - X_n]$ indicating the input vector containing n features, and Y $takes\ the\ value\ Y_1 - Y_n]$ represents the vector containing n transformed values.

3. Design of Algorithms

For examining STEM picture of a nano substance, researcher suggested an approach called ML for ML-SIA. Researcher suggested yet another approach for processing spectrum data of STEM image for nano material called ML for ML-SISDA. A prototype ML application was created for implementing the algorithms & assess the suggested approach.

Algorithm 1: STEM Image Analysis (ML-SIA)

```
Step 1: Start
Step 2: Extract Features (STEM image of an oxide catalyst [I])
Step 3: For each ML technique t in P
Step 4: TrainClassifier (Training data T)
Step 5: FitModel(M,F,I)
Step 6: Display STEM image analysis
Step 7: End For
Step 8: End
```

As shown in Algorithm 1, different ML models, like SVM and DT, are used to classify the given STEM picture. The training data T, the workflow of these models, and the STEM picture for an oxide catalyst are the components that constitute the program. STEM picture analysis and data are given through a process that repeats itself. Another suggested method is ML-SISDA.

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

```
Step 1: Start
Step 2: Initialize results list R
Step 3: Extract Spectral Data from image I
Step 4: Iterate Over Machine Learning Models in set P:
Compute r = Apply Spectral Data Analysis on Spectral using model m
Store r in R
Step 6: End Loop
Step 7: Display Results stored in R
Step 8: End
```

As shown in Algorithm 2, it delivers the outcomes of the analysis of the STEM image spectral data after receiving as inputs a STEM picture of an oxide catalyst and a pipeline of ML models. It extracts the supplied image's spectral characteristics. After that, it uses an iterative procedure to analyze spectrum data from various angles and provide visual representations of the data for nanomaterial characterization. This is the machine learning strategy that might advance the field.

4. Results and Discussion

This section demonstrates the experiment findings for the suggested method, which includes analyzing STEM images and spectral data from a picture of a nanomaterial. As an example, a STEM picture taken from a nanomaterial related to an oxide catalyst is used to test the suggested methods. For the actual study, various machine learning methods are utilized. Some of them are n-FINDR, NMF, ICA, DT, and SVD in order. The outcomes are split into STEM picture analysis results as well as STEM spectral data analysis results.

4.1. Outcome of STEM Image Analysis

A STEM image taken from a nanomaterial related with an oxide catalyst is characterized and analyzed using two well-known machine learning methods, SVM and DT. When it comes to analyzing and creating the necessary classes, the two categorization models do use distinct methodologies. The analysis is conducted using two classifications.

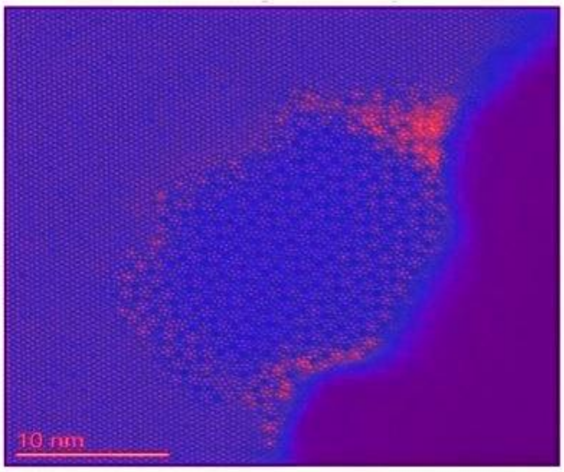

Figure 2a STEM Image of Oxide Catalyst.

As shown in Figure 2a, it shows a STEM image of an oxide catalyst. The properties of nano materials are known via scanning transmission electron microscope imaging technique.

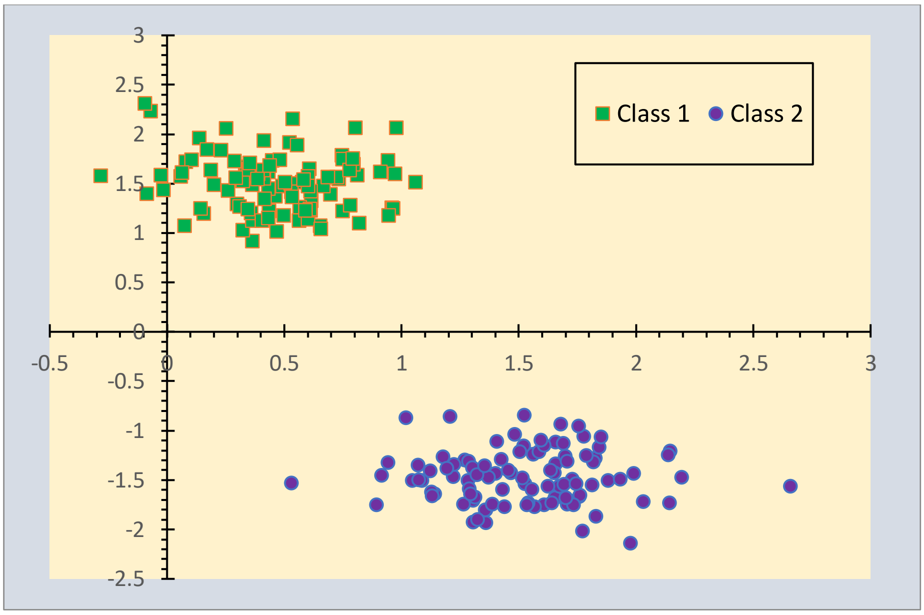

Figure 2b Outcome of SVM Classification.

The outcome of SVM classification for the STEM image is shown in Figure 2b. Based on SVM's hyperplane for classification, it is binary classification which has produced two classes. The line graph illustrates a classification issue in which two distinct data point classes are represented in two dimensions, with a decision border separating them. Class 1 and Class 2 data points are scattered in the top and bottom regions of the graph, respectively, with green and violet dots, respectively, indicating the two categories. Measurable attributes utilized for categorization are represented by the x-axis for Feature X & the y-axis for Feature Y. Each point in top portion is categorized as Class 1, whereas any point below in the bottom portion is classed as Class 2, according to the equation for this decision boundary, which is $y = x - 0.5$.

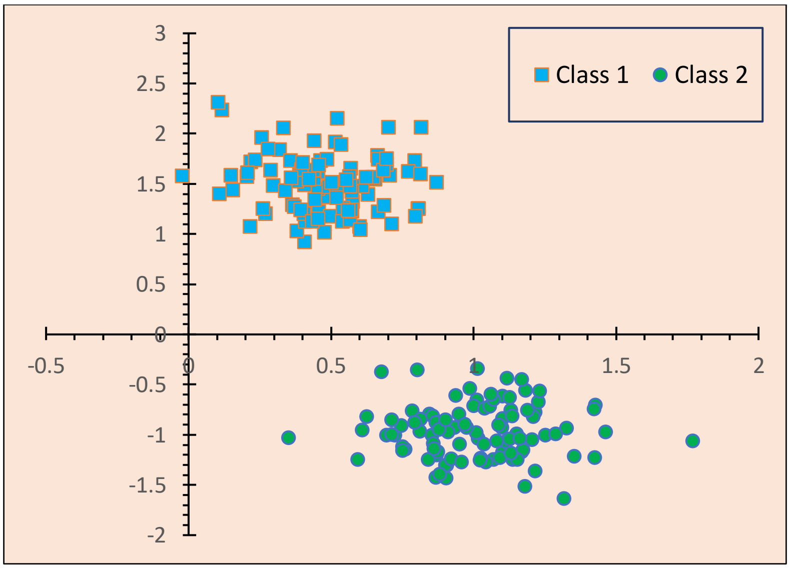

Figure 2c Outcome of Decision Tree.

Figure 2c depicts classification outcome done by Decision Tree method with two classes. This categorization is dependent on the DT algorithm's capacity to detect attribute for splitting. The figure shows how the model sorts the data into groups. Additionally, there doesn't seem to be a clear line between the two classes because most of the points are correctly labelled. But sometimes incorrect classes are chosen, especially near the edge where data points meet or close to each other.

4.2. Outcome of Spectral Data Analysis

A STEM picture is utilized as input, and several techniques are employed for spectral data processing. The empirical investigation was conducted using SVD, NMF, ICA, and n-FINDR as methodologies.

It can be seen in Figure 3(a) that the sliding window method is used with FFT windows to analyze spectral data. The FFT visualization containing multiple datasets is shown in the provided image. An image's periodic patterns, noise, as well as frequency components may all be examined with the use of the FFT, a mathematical tool that transforms data from the spatial domain to the frequency domain. Each subplot represents a distinct FFT transformation performed to various picture patches or datasets, and the image is organized in a 3x3 grid containing nine FFT representations designated Alt FFT 0 to Alt FFT 8. A purple-to-red colormap, probably called "plasma" is used for the color representation in order to improve viewing. High-intensity frequency components, that might show dominating frequencies in the original picture, are indicated by the bright yellowish dots in certain graphs.

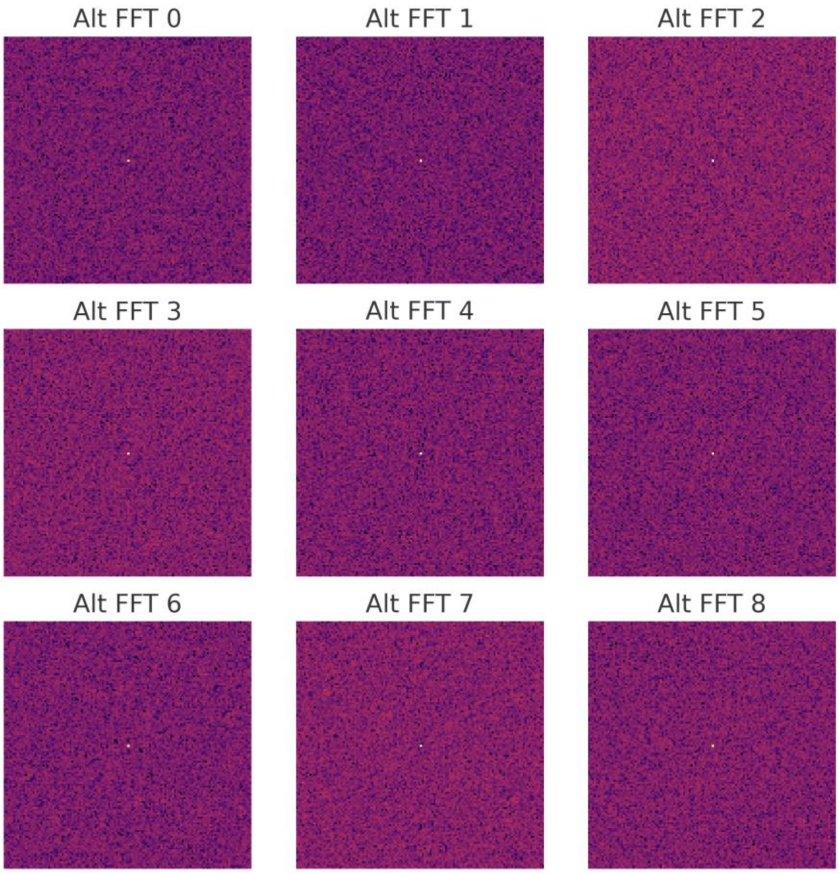

Figure 3a Analysis of Spectral Data with FET.

In frequency analysis, the low-frequency parts are usually found in the middle of the FFT plots, while the high-frequency parts are found on the edges. Perhaps repeated patterns or organized noise in the source pictures caused the bright spots that stand out on their own. The rest have a more even distribution, which could mean absence of clear repeated structures. Some FFTs have a brighter area that is more concentrated, which means that the periodic patterns are greater.

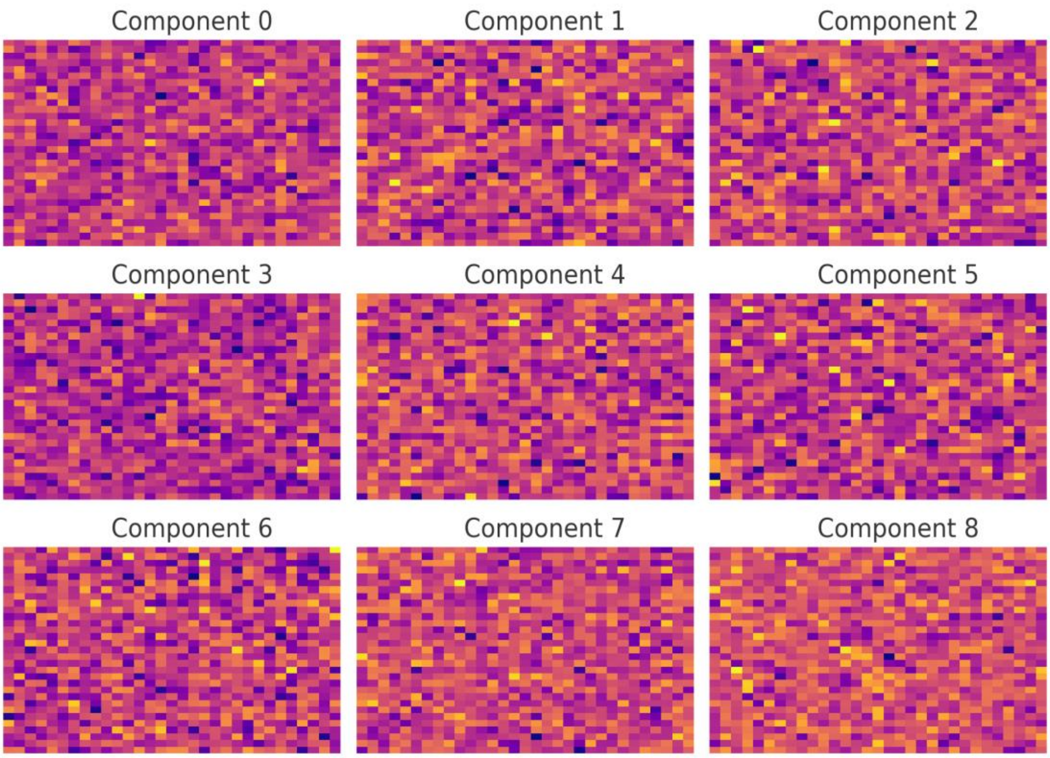

Figure 3b Analysis of Spectral Data with SVD Abundance Maps.

The SVD abundance maps in Figure 3b are used for examining at spectral data. Different parts of the image show how SVD abundance maps are visualized and are used to find the spectral data linked to a certain STEM. The distribution of specific patterns throughout the data is shown by each of the nine subplots, which correspond to various main components. On a scale from very dark purple to very light yellow, the color intensity shows how much of a certain component there is in various areas. Differences in pattern interpretation across the subplots provide insight on the relative importance of the dataset's structural, spectral, and spatial properties.

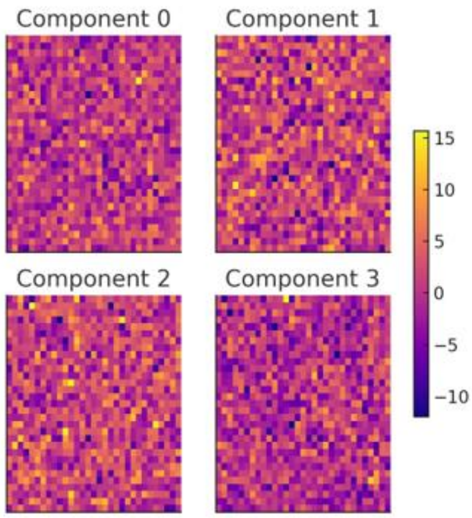

Figure 3c Analysis of Spectral Data with NMF Abundance Maps.

Numbers from the NMF can be used to make maps of NMF abundance, as shown in Figure 3(c). The Non-negative Matrix Factorization (NMF) Abundance Maps are used for finding the important traits from a dataset. They are most often used in material analysis or hyperspectral images. Each of the four subplots in the picture represents an NMF-extracted component. Along with assisting to find underlying spectral fingerprints or regional distributions, these parts bring out clear patterns and structures in the data. It's clearer to identify the difference between areas now that a plasma colormap have been used to increase contrast. The lightest shades show higher intensities, and the darkest shades show lower intensities. The color bar in the right shows the range of abundance numbers.

5. Conclusion

A ML based approach for analyzing STEM images as well as spectral data from nanomaterial STEM images was presented in this study. ML-SIA is the approach researcher suggested for analyzing STEM images of nanomaterials. Additionally, researcher suggested a different approach for analyzing the spectrum data of STEM images of nanomaterials called ML-SISDA. To take advantage of the algorithms and assess the suggested approach, researcher created a prototype machine learning application. Experimental findings indicated that the ML based techniques are beneficial for the characterization of nano materials. Therefore, by starting further work on the field of material analysis using artificial intelligence, this study advances ahead. To get more out of characterizing nanomaterials, researcher plan to examine the DL models on nanomaterial research in the future. In terms of quality and efficiency, this will help many fields, such as the storage device production industry.

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