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REGULAR ARTICLE

Automated Classification of Carbon Nanomaterial Structures based on Computer Vision Model

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Carbon nanomaterial structures hold significant promise across various industries, necessitating accurate and automated classification methods. Conventional approaches rely on handcrafted feature extraction techniques, often failing to capture complex spatial patterns inherent in nanostructures. Traditional Machine Learning (ML) and basic Deep Learning (DL) models suffer from low generalization and require manual feature engineering, making them inefficient for handling diverse and noisy microscopy images of nanostructures. The objective is to achieve a highly accurate and automated classification of carbon nanomaterial structures through an advanced framework. A novel approach Modified Water Wave-inspired Convolutional Autoencoder with Swin Transformer (MWW-CAE-ST), integrates optimization, and classification techniques to address existing challenges. A collection of microscopy images of carbon nanomaterials, including diamond particles, and nanotubes was used to evaluate the framework. Techniques, such as median filtering and histogram equalization (HE) were applied to enhance image quality by reducing noise and normalizing intensity levels. Local Binary Patterns (LBP) were employed to extract texture-based features that capture fine-grained details of the nanomaterial structures. Features generated by LBP were processed through the CAE for dimensionality reduction and refined by the Swin Transformer, which utilizes hierarchical self-attention to classify structures effectively.

Keywords: Carbon nanomaterials, Microscopy image analysis, Modified water wave optimization, Convolutional autoencoder (CAE), Swin transformer.

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1. INTRODUCTION

Advanced scientific and technological applications expect these essential carbon nanomaterial structures because their nanoscale carbon atomic arrangements present outstanding mechanical, electrical, and thermal properties [1]. Carbon nanomaterials consist of five diverse structures, which include fullerenes as well as carbon nanotubes (CNTs), graphene, nanodiamonds and carbon nanofibers. Each has its molecular structure and specific properties. The broad application of nanotechnology depends on their exceptional strength level combined with high electrical conductivity properties and superior thermal stability features [2]. The carbon nanomaterial classification based on dimensionality is shown in Fig. 1.

Carbon nanomaterials demonstrate flexibility in environmental applications for water purification and gas absorption processes [3]. At present nanoscience remains active and these materials maintain outstanding potential to advance both manufacturing sectors and generate miniature electronic devices while fueling the development of new battery designs and medical treatment methods, thus guiding the path of material science and engineering into the future [4]. Carbon nanomaterial structures encounter multiple obstacles during scalability, defect regulation, cost efficiency and stability, reproducibility, environmental risks, toxicity effects, and integration difficulties. Hence The MWW-CAE-ST approach seeks to accomplish automatic carbon

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nanomaterial classification at high accuracy through the integration of optimization and DL.

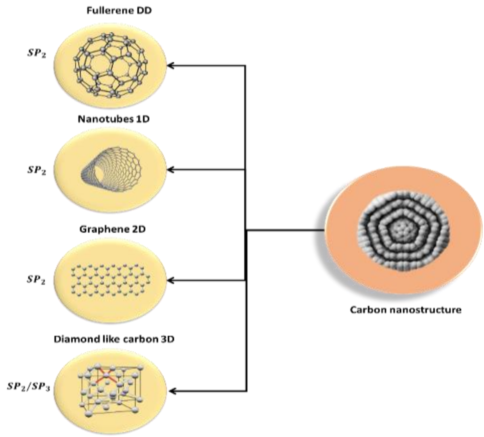

Fig. 1 – Carbon nanomaterial classification based on dimensionality

Convolutional Neural Network (CNN)-based ML with computer vision for categorizing and identifying Carbon Nanotube/Carbon Nanofiber (CNT/CNF) particles present in Transmission Electron Microscopy (TEM) images is presented in [5]. The classification methodology achieved 90.9 % accuracy for the 4-class data while dealing with an 8-class dataset and obtained 84.5 % accuracy. The importance of ML technology for nanomaterial design through analysis of seven perspectives over quantitative analysis was explored in [6]. The scientific understanding of nanomaterial design needed valuable data because it sustained and accelerated material innovation development.

The DL technology was applied to Raman imaging to develop an efficient method for carbon nanotube (CNTs) detection and characterization in [7]. The result revealed that the adaptability of nanoparticles during manufacturing processes evaluated the material quality and characteristics while production occurs. Carbon nanomaterials, which enable electrochemical point-of-care devices that use aptamers to detect cancer, were discovered in [8-9]. The result focused on a tamers that were directed against potential cancer-related biomarkers. The investigation stressed both the prospects of connecting bio-sensing devices with Internet of Things (IoT) platforms.

A combined approach based on ML to forecast the thermal conductivities of Polymeric Nanocomposites (PNCs) was discussed in [10-11]. It improved the hybrid intelligence algorithm for predictions, which resulted in superior performance compared to standard neural networks. ML together with meta-analysis to develop predictive models that determined protein corona structure and cellular recognition patterns of Nanoparticles in [12]. The approach served as helpful in predicting the functional properties of the protein corona that determined cellular recognition because it enabled the direction of NP synthesis and application. DL techniques help to identify metal nanoparticles on highly orientated pyrolytic graphite through automated analysis of Scanning Tunneling Microscopy (STM) images as described in [13].

2. METHODOLOGY

At the beginning of the investigation, the microscopic images of carbon nanomaterials including diamond particles and nanotubes were collected. The procedure requires the application of median filtering and HE techniques to microscopy images for noise reduction purposes along with intensity normalization steps. The LBP method first extracts texture attributes before passing them through CAE to reduce data dimensions. ST performs feature refinement alongside MWW, which optimizes hyper parameters to boost accuracy together with operational effectiveness.

2.1 Dataset

The training and testing of the automated classification system occur through images obtained from microscopy. The Diamond Particles and Carbon Nanotube Images dataset contains TEM images that show nanomaterials through diamond particles and carbon nanotubes. The dataset functions as a vital exploration tool for improvements in nanotechnology together with microscopy image analysis and computational material science.

2.2 Data Pre-Processing

Pre-processing improves image quality while removing noise, normalizing intensity values and extracting significant texture characteristics suitable for classification. Image clarity enhancement came through median filtering for noise removal together with HE for intensity normalization during data pre-processing.

2.2.1 Median Filtering

It cleans image noise to defend nanomaterial edges so feature extraction can be carried out precisely. A non-linear filter called a median filter regulates the median of the set of pixels that are inside the filter mask. The statistical median of each pixel's $M \times N$ neighborhood is used to swap it. Because the median value is derived from the neighborhood pixel, edge blurring and image detail loss are conserved because it is more robust to outliers and does not afford a new accurate pixel value. Sharp regularity structures are conserved. As the gap size increases, the median filter's capacity to decrease noise rises as well. The median filter formula is given in Equation 1.

$$e(w, z) = \{h(t, s)\} \tag{1}$$

Where T_{WZ} signifies the $M \times N$ sub-image window's coordinates.

2.2.2 HE

The method improves imaging clarity since it regularizes intensity distribution, allowing observing nanomaterial structures. Examine a digital image that has greyscale principles between $[0, K-1]$, Probability Circulation Equation (2) can be used to estimate the image's function:

$$O(q_l) = \frac{m_l}{M} \quad l = 0, \ldots\ldots, K-1 \tag{2}$$

Where m_l is the sum of pixels and q_l is the lth old level of the image's pixels with the old levelq_l .

Another process for calculating the Cumulative Distribution Function (CDF) is as follows in equation 3.

$$D(q_l) = \sum_{j=0}^{j=l} \quad O(q_j) \quad l = 0, \ldots., K-1,\ 0 \le D(q_l) \le 1 \tag{3}$$

Using equation (3), HE alters the input image's old level T_l to old levelq_l. Thus, equation 4 as follows.

$$T_l = (K-1) \times D(q_l) \tag{4}$$

The standard HE method can be used to estimate the variations in old level T_l in equation 5.

$$\Delta T_l = (K-1) \times O(q_l) \tag{5}$$

Equation (5) specifies that the input image at old level q_l is directly connected to the distance between T_l and $T_l + 1$. Due to the quantization process and briefing aspects of equation (3), unwanted effects of the standard HE approach be formed.

The image was processed through the median filter and HE is shown in Fig. 2.

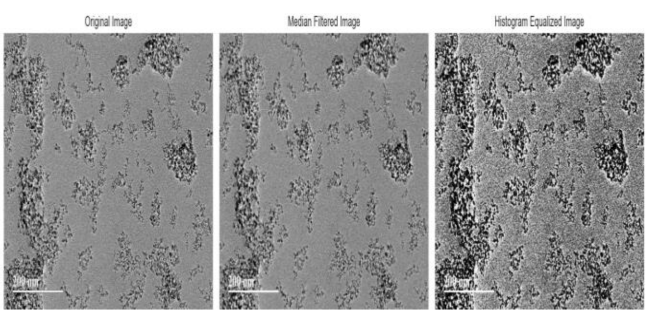

Fig. 2 – Visual representation of image processed through Median Filter and HE

2.3 LBP

Texture elements within carbon nanomaterials get noticed. The image extraction through LBP is shown in Fig. 3.

2.4 MWW-CAE-ST

MWW-CAE-ST serves as a combination of optimization algorithms along with feature extraction and classification methods dedicated to carbon nanomaterial images. MWW optimizes hyperparameter settings and determines the most suitable features to achieve better efficiency. The CAE reduces system dimension while conserving significant textures within its framework. Feature representation along with classification accuracy receives enhancement from hierarchical self-attention through ST. Such a combined analytical process offers optimal performance together with high processing speed and extended scalability capabilities in nanostructure analysis.

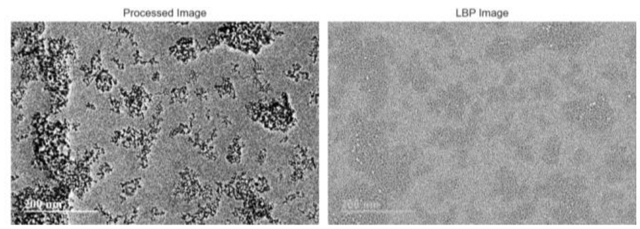

Fig. 3 – Visual representation of image extraction through LBP

2.5 ST

ST represents the naming scheme for carbon nanomaterial structures because it uses hierarchical self-attention mechanisms to classify. The ST is one of the most significant enhancements made to the Vision Transformer design. In deeper layers of the model, the image patches are combined to create hierarchical feature maps. The computational cost is linear concerning the size of the input image. It engages in self-attention within each local window, which explains this behavior. As a result, it can be considered a broad framework for managing tasks involving object identification or image classification. The old vision transformers compute attention to overall points in the input image at a quadratically high cost and provide latticed feature maps with only one level of resolution. Swin Transformer-based image processing flow is shown in Fig. 4.

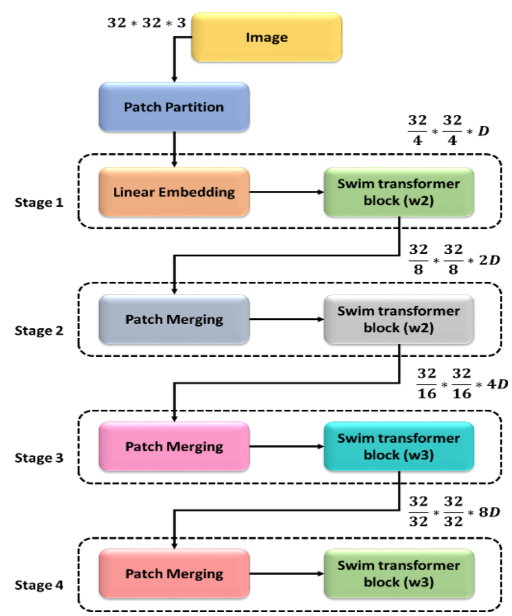

Fig. 4 – Swin transformer-based image processing flow

Transformer Swin Each level of this ST architecture is made out of a group of blocks. These blocks consist of feedforward neural networks and several layers of attention. The ST is divided into four stages, each of which consists of an ST block and Linear Embedding, as well as a Patch Partition. Patch merging over applies the ST block in the final three steps. Each of these description components can be found below. As envisioned in this investigation, the suggested architecture uses a combination of enhancers and STs to provide sufficient information to determine whether images have undergone even the slightest alteration: that are categorized as fake and deviate from the state with any degree of certainty.

2.6 CAE

The CAE-ST tool pulls out, shortens, and sorts texture features, which leads to the exact recognition of carbon nanomaterial structures. Convolutional layers make up CAEs, which are unverified dimensionality reduction algorithms that can produce compacted image representations. CAEs are used predominantly to remove robust features, reduce and compress the input dimension size, and eradicate noise while recollecting all relevant information. The use of convolutional layers is the main difference between convolutional AE and standard AE. It is significant to note that these layers are notable for the attractive skill of learning interior demonstration of image data and extracting knowledge. The decoder, is in charge of reconstructing the compacted latent representation so that the last image is as equal to the original as possible. The architecture of a CAE is shown in Fig. 5.

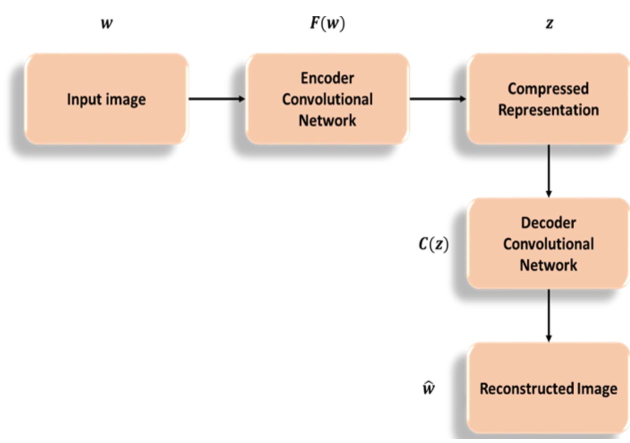

Fig. 5 – Architecture of a convolutional autoencoder (CAE)

3. RESULT

In the present investigation, Windows 11 is selected for implementation, having an Intel i5 7th Gen processor and 16 GB RAM installed in the computer. Automated classification of carbon nanomaterial structures and optimization will be conducted using Python 3.10.1 and a DL technique known as "MWW-CAE-ST". These evaluations find their use in the assessment of the algorithm through accuracy and F1 Score.

This model proves effective in carbon nanomaterial classification through its final accuracy score. The MWW-CAE-ST successfully extracts crucial features followed by their refinement process to achieve robust classification of various microscopy images. The framework proves suitable for automatic nanomaterial identification tasks, because it demonstrates both high accuracy and versatility in classification. The training and validation accuracy for the model is shown in Fig. 6.

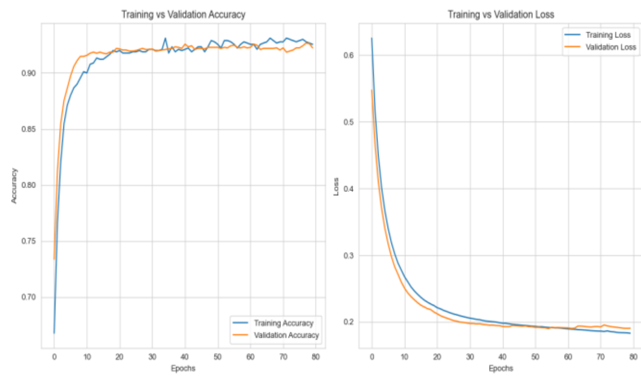

Fig. 6 – Training vs. Validation performance: accuracy and loss trends

3.1 Accuracy

Classification performance of carbon nanomaterial structures obtained from microscopy images through the accuracy. It defines the percentage of instances properly classified among the total number of samples. The proposed MWW-CAE-ST model surpassed the custom network with 92.3 % accuracy while achieving 77.1 % accuracy. It shows that higher accuracy makes a robust, efficient, and reliable solution for carbon nanomaterial classification. Table 1 and Fig. 7 represent the comparison of accuracy between models.

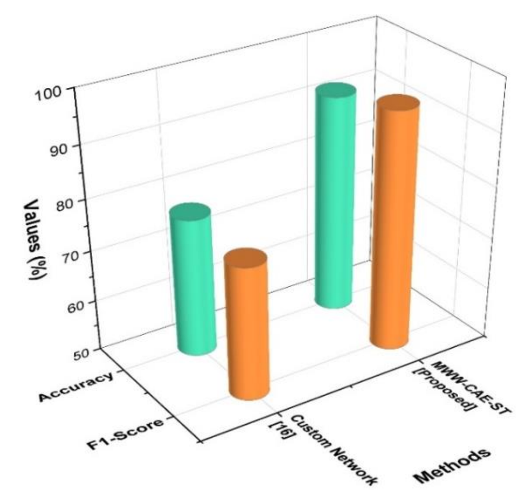

Fig. 7 – Comparative analysis of accuracy and F1-score between custom network and MWW-CAE-ST

3.2 F1 Score

It evaluates classification results with equal importance for precision ratings together with recall metrics. The F1-Score parameter combines precision with recall, since these values matter most for data that contains uneven distribution. The custom network achieved a 76 % F1-Score but MWW-CAE-ST produced a 96 % F1-Score, which indicates that the latter method delivers superior predictive abilities.

4. CONCLUSION

Carbon nanomaterial structures include nanoscale materials that involve nanotubes along with Nano spheres and Nano fibers, which possess distinctive mechanical and electrical features. The dataset contains images of diamond particles and nanotubes among carbon nanomaterials. LBP serves as the extraction method that detects detailed texture information to produce effective nanomaterial structure representations for classification purposes. The MWW-CAE-ST model demonstrates superior performance compared to the traditional model because it delivers 92.3% accuracy combined with a 96% F1-score and achieves improved classification and generalization together with enhanced feature extraction. The proposed model maintains high accuracy, but exists with some implementation challenges. Future exploration should address three main challenges, it should simplify computational demands, improve resistance to various imaging environmental changes, and explore self-supervised learning to improve generalization abilities.

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Автоматизована класифікація структур вуглецевих наноматеріалів на основі моделі комп'ютерного зору

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Структури вуглецевих наноматеріалів мають значні перспективи в різних галузях промисловості, що вимагає точних та автоматизованих методів класифікації. Традиційні підходи спираються на ручні методи вилучення ознак, які часто не в змозі вловлювати складні просторові закономірності, властиві наноструктурам. Традиційні моделі машинного навчання (ML) та базового глибокого навчання (DL) мають низький рівень узагальнення та вимагають ручної розробки ознак, що робить їх неефективними для обробки різноманітних та шумних мікроскопічних зображень наноструктур. Метою є досягнення високоточної та автоматизованої класифікації структур вуглецевих наноматеріалів за допомогою вдосконаленої структури. Новий підхід, натхненний модифікованими водяними хвилями, згортковим автоенкодером із трансформатором Swin (MWW-CAE-ST), інтегрує методи оптимізації та класифікації для вирішення існуючих проблем. Для оцінки структури було використано колекцію мікроскопічних зображень вуглецевих наноматеріалів, включаючи алмазні частинки та нанотрубки. Для покращення якості зображення шляхом зменшення шуму та нормалізації рівнів інтенсивності було застосовано такі методи, як медіанна фільтрація та вирівнювання гістограми (HE). Для вилучення текстурних ознак, які фіксують дрібнозернисті деталі структур наноматеріалів, було використано локальні бінарні шаблони (LBP). Ознаки, згенеровані LBP, були оброблені за допомогою CAE для зменшення розмірності та уточнені за допомогою Swin Transformer, який використовує ієрархічну самоувагу для ефективної класифікації структур.

Ключові слова: Вуглецеві наноматеріали, Аналіз мікроскопічних зображень, Оптимізація модифікованої водної хвилі, Згортковий автоенкодер (CAE), Трансформатор Swin.