Multi-Modal Nanomaterial Characterization: Integrating SEM/TEM Imaging with LLM-based Text Understanding

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Abstract. Nanomaterials characterization has historically utilized high-resolution imaging methods, such as Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM), to obtain information on the structural and morphological characteristics of nanomaterials. SEM and TEM are limited in their ability to provide useful contextual information about the nanomaterial being characterized. Relevant contextual information can include details about the synthesis of the material, as well as the precise chemical composition and other annotations regarding the material's potential use. Characterizing nanomaterials using a single imaging modality limits the ability to accurately classify and understand nanomaterial morphology and composition, and therefore develop accurate methods for synthesizing nanomaterials. The multimodal nanomaterial characterization system proposed will provide an alternative approach to overcome the above limitations by combining the structural and morphological information from the images, with the contextual information. More specifically, a convolutional neural network will be used to encode the images with a transformer-based language model trained on scientific articles for the purpose of encoding the contextual information about the nanomaterials. Subsequently, the proposed model will integrate these two types of information using a cross-modal attention mechanism to create enriched multimodal embeddings for classification purposes. The proposed Retrieval-Augmented RoBERTa–based multimodal system is experimentally verified over 3,501 SEM/TEM image–text pairs to have a classification accuracy of 92.02% and a macro F1-score of 0.8288. More importantly, this approach was able to improve the recognition capability of underrepresented nanoparticle morphologies with a 65% relative increase in F1-score pertaining to the minority "triangle" class with respect to baseline multimodal models. Hence, the multimodal characterization system has the potential to provide a scalable method for automating the analysis of nanomaterials for quality control, high-throughput screening and material discovery.

Keywords: Multimodal learning · nanomaterial characterization · SEM · TEM · transformer · image-text fusion

1 Introduction

Recent developments in nanotechnology have created an increasing need for rapid and automated methods for nanomaterials characterization. The physical and chemical characteristics of nanostructures, like morphology, crystallinity, and composition, have a direct impact on their electronic, catalytic, and even biomedical behavior. Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM) have been widely employed to examine these parameters, yielding high-resolution structural information across various spatial dimensions [1], [18]. The rapid growth of microscopy imaging data produced by modern laboratory instruments has made traditional manual analysis strategies inadequate.[5] [12] For this reason, machine learning (ML), particularly deep learning (DL), has emerged as the revolutionary paradigm for the autoproduction of image-based feature extraction, classification, and pattern discovery of nanomaterial data [5], [6]. However, most of the present works are unimodal, solely relying on visual data acquired through SEM/TEM imaging and ignoring relevant auxiliary metadata, i.e., synthesis conditions, chemical compositions, fabrication parameters, or material labels [12], [16]. These textual annotations frequently furnish essential semantic information that enhances feature interpretability and augments predictive accuracy.[9] [26]

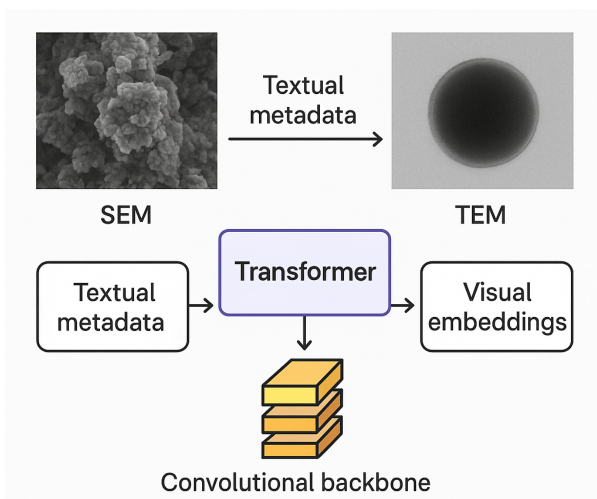


Fig. 1: Overview of the multimodal nanomaterial characterization system integrating SEM/TEM image features with textual embedding.

To overcome this limitation, multimodal learning provides a viable avenue by trading-off between heterogeneous data sources [1], [2]. By simultaneously learning from visual and textual modality (scientific description, procedures for synthesis, annotations), multimodal models are able to construct richer feature representations, improve generalization, and provide more robust classification and characterization of nanomaterials [7], [13]. The proposed study investigates such an integrative deep learning system fusing SEM/TEM imagery and scientific text embeddings. At present, these two data types—image data and descriptive data—are analyzed as separate data sources and their combined contributions to the characterization and classification of nanomaterials is less optimal. The development of a multimodal approach that can connect visual information from SEM/TEM images and contextual knowledge acquired from extracting information from text through pre-trained models such as BERT may allow for an automated, accurate, and explainable approach to the characterization of nanomaterials [1], [4].

Traditional unimodal CNN-based models and handcrafted feature extraction pipelines have been used for nanomaterial analysis, but they fail to exploit textual metadata [5], [6]. Vision-only transformers improve representation but still lack semantic grounding [7], [8]. Our approach bridges this gap by incorporating multimodal fusion [14].

The major objectives and contributions of this work is as follows:

(i) To develop a multimodal deep learning system that fuses SEM/TEM image features with scientific text embeddings. [1] [4]
(ii) To improve the accuracy, interpretability, and robustness of nanomaterial classification [13].

This paper is organized as follows. Section 2 reviews the state-of-the-art literature in three focal areas: deep learning approaches for the analysis of SEM/TEM images, transformer-based large language and vision-language models, and techniques regarding multimodal fusion for nanomaterial characterization. Section 3 elaborates on the proposed multimodal work, starting with the preprocessing steps, fusion mechanisms, classification and evaluation protocols. The results of the experiments are presented in Section 4, where models and their variants are examined, including comparisons of their performances. Lastly, Section 6 summarizes our conclusions and discusses opportunities for further research in fine-grained property prediction, self-supervised learning, and real-time decision support systems.

2 Literature Review

Traditionally, nanomaterials have been characterized by SEM and TEM, where particle morphology, size distribution, and surface topology are measured. Scientists publish a huge amount of helpful information in their papers, especially in things like figure captions and experiment steps. But most automated tools don't take full advantage of this rich information yet.[12] [16].

Initial automation efforts in microscopy employed CNNs for segmentation of nanoparticles, estimation of size, and morphological classification. Mourdikoudis et al. [1] stated that despite SEM and TEM obtaining excellent spatial resolution when characterizing nanoparticle morphology in terms of size and shape relationships are best used in conjunction with compositional approaches as part of an overall composite measurement.

Self-supervised microscopy, generative methods and crossmodal transformers for visual-text fusion made electron microscopy analysis better in more studies.[11]-[16] Even with these improvements, the lack of standardized benchmarks and limited cross-instrument generalization still make it hard to scale models. Meanwhile, advances in image-based methods have been matched by significant advances in the textual modality, enabled by transformer-based architectures. Transformer models, such as BERT[1] and GPT-3[3], have allowed for contextual learning and few-shot adaptability. Within materials science, Yu [4] showed that fine-tuning LLMs on domain-specific corpora accelerates discovery in a wide range of domains. Aside from text, Vision–Language Models (VLMs) such as CLIP and NatureLM [10] integrate semantic and visual understanding through cross-attention mechanisms. Ghosh [7] and Jeong [8] also looked at domain adaptation techniques under scientific and medical imaging, emphasizing the challenge through the application of general-purpose models on microscopic data. Lai [9] and Weng et al. [13] contributed benchmark datasets presenting first baselines to measure multimodal performance through materials science.

During the past two years, a number of developments have further accelerated progress in both multimodal and microscopy-focused applications. Retrieval-augmented generation frameworks and domain-specific fine-tuning of large language models are increasingly applied to materials science to provide external knowledge due to the scarcity of annotations, reflected in recent surveys and domain LLM studies.[4] [10] Adaptation of vision–language models and cross-attention fusion mechanisms for microscopy images has shown early success for the alignment of structural image features with scientific textual descriptions.[7][8] [14] A set of self- and semi-supervised learning strategies for electron microscopy improve robustness under limited labeling, and new evaluation standards have emerged in terms of benchmarks and datasets that are specific to materials characterization.[9]. Cross-attention rooted fusion models, i.e., CAST by Lee et al. [14], suggest the potential of structure-text embedding alignment towards property prediction. Falke et al. [10] offered an extensive overview on the characterization and classification of nanoparticles, making the case that single-modality strategies necessarily confine the depth of knowledge obtainable with the analysis of nanomaterials. Miguel et al. [11] reviewed synthesis and characterization of nanomaterials for electrochemical purposes, showing that integration of structural imaging with compositional and textual metadata supports more stable characterization results than individual analysis strategies. None of the above works tend to integrate RAG-style retrieval with cross-modal attention for SEM/TEM image–text fusion for morphology classification—a gap this work seeks to address.

Hence, the work here builds upon these results by proposing the CNN + LLMs-Based multimodal model that combines SEM/TEM image-derived spatial representations and contextual embeddings from domain-trained language models to boost interpretability and reduce the necessity to depend on manual expertise.

3 Methodology

The technique successfully classifies nanomaterials using a combination of text and visual data. A detailed flowchart of the working procedure is displayed in Fig. 2.

3.1 Experimental Workflow

The experimental pipeline comprises seven sequential stages summarized below.

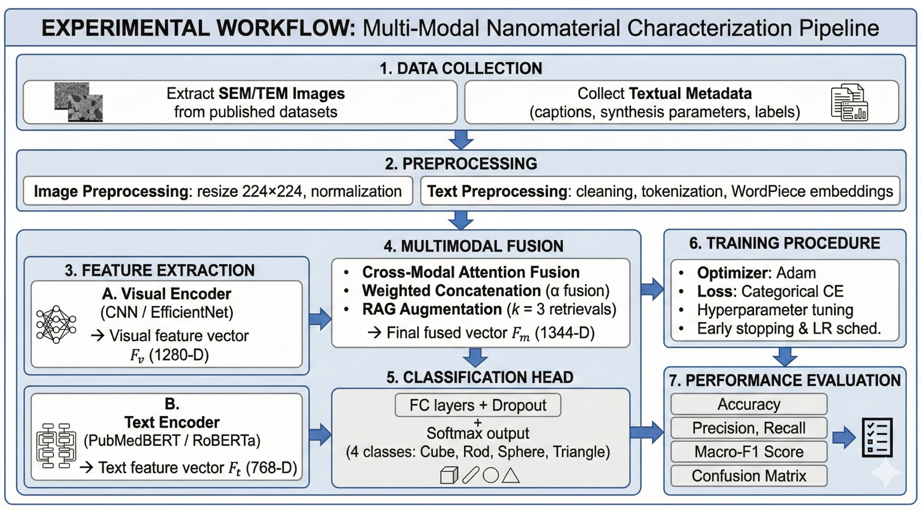


Fig. 2: The methodological pipeline delineates dataset preprocessing procedures, feature extraction utilizing CNN and BERT architectures, multimodal fusion strategies, and subsequent classification with performance evaluation.

(i) **Data collection.** To develop the dataset for the classification models, SEM/TEM microscopy images are used from the published literature, extracted using a fully automated pipeline. The dataset with experimental images generated on TEM images, making sure all the images were matched with domain-specific annotations that included morphological classifications, parameters for the synthesis, and material compositions. The ground-truth labels for the four nanoparticle morphologies into one-hot encoded vectors.[17]

(ii) **Data preprocessing.** The images are all resized, for instance, 224×224, and normalized using ImageNet [2]. Text annotations are lowercased, de-noised (removal of boilerplate and non-informative tokens), tokenized, and encoded using subword methods (e.g., WordPiece).

(iii) **Feature extraction.** The spatial representations are obtained from SEM/TEM images using a pre-trained CNN, such as EfficientNet, and textual features are obtained from a transformer encoder (e.g., BERT or SciBERT) [1] using CLS embedding as the textual descriptor $\mathbf{F}_t$.

(iv) **Multimodal fusion.** The principal contribution of this work lies in the efficient integration of visual and textual modalities within a unified multimodal representation. Let $\mathbf{F}_v \in \mathbb{R}^{d_v}$ denote the visual feature vector extracted from SEM/TEM images and $\mathbf{F}_t \in \mathbb{R}^{d_t}$ denote the textual feature vector extracted from scientific annotations, where $d_v = 1280$ and $d_t = 768$ are the respective feature dimensions.

Cross-Modal Attention Fusion The cross-modal attention mechanism aligns the visual and textual representations for attention weights conditioned on the visual modality:

$$\text{Attention}(\mathbf{F}_v, \mathbf{F}_t) = \text{Softmax}\left(\frac{\mathbf{QK}^\top}{\sqrt{d_k}}\right)\mathbf{V} \tag{1}$$

The cross-attended textual representation is concatenated with visual features:

$$\mathbf{F}_m = \text{Concat}(\mathbf{F}_v, \text{Attention}(\mathbf{F}_v, \mathbf{F}_t)) \in \mathbb{R}^{d_m} \tag{2}$$

Weighted Concatenation Baseline A computationally cheaper weighted fusion is also used:

$$\mathbf{F}_m^{\text{weighted}} = \alpha \cdot \mathbf{F}_v + (1-\alpha) \cdot \mathbf{F}_t \tag{3}$$

with learnable $\alpha \in [0, 1]$.

Retrieval-Augmented Generation (RAG) Enhancement The RAG variant augments the multimodal representation using retrieved contextual information from a knowledge base $\mathcal{K}$[3]:

$$\mathbf{R}(\mathbf{F}_t) = \text{Retrieve}(\mathbf{F}_t, \mathcal{K}, k = 3) \tag{4}$$

The RAG-augmented fusion is:

$$\mathbf{F}_m^{\text{RAG}} = \beta\mathbf{F}_m + (1-\beta)\mathbf{R}_{\text{agg}}(\mathbf{F}_t) \tag{5}$$

where $\beta \in [0, 1]$.

(v) **Classification Head.** The fused representation $\mathbf{F}_m$ is processed through a fully connected layer with dropout:

$$\mathbf{h}_1 = \text{Dropout}(\text{ReLU}(\mathbf{WF}_m + \mathbf{b}), p_{\text{drop}}) \tag{6}$$

The final prediction is:

$$\hat{\mathbf{Y}} = \text{Softmax}(\mathbf{Wh} + \mathbf{b}) \in \mathbb{R}^C \tag{7}$$

with $C = 4$ nanoparticle classes.

(vi) **Training and evaluation.** Adam optimizer is used with cross-entropy loss. For each class $c \in \{1, 2, 3, 4\}$:
a) Precision:

$$\text{Precision}_c = \frac{\text{TP}_c}{\text{TP}_c + \text{FP}_c} \tag{8}$$

b) Recall:

$$\text{Recall}_c = \frac{\text{TP}_c}{\text{TP}_c + \text{FN}_c} \tag{9}$$

e) Macro F1-score:

$$\text{F1}_{\text{macro}} = \frac{1}{C} \sum_{c=1}^{C} \text{F1}_c \tag{10}$$

g) Accuracy:

$$\text{Accuracy} = \frac{\sum_{c=1}^{C} \text{TP}_c}{\sum_{c=1}^{C} (\text{TP}_c + \text{FN}_c)} \tag{11}$$

3.2 Model Variants

To test the proposed multimodal framework, we came up with three different model setups, which are detailed below.

(i) *Multimodal PubMedBERT:* The variant employs the PubMedBERT language encoder, which is pretrained only on biomedical and scientific articles, to produce the particular textual embeddings.

(ii) *Multimodal RoBERTa:* RoBERTa transformer as the textual encoder considered in this interplay due to its powerful contextual modeling and being the best on large general-domain datasets. Its inclusion with image features will make the learning of the multimodal representation much stronger. This approach facilitates enhanced generalization capabilities that transcend domain-specific constraints.

(iii) *Multimodal RoBERTa with Retrieval-Augmented Generation (RAG):* The model with RAG is given a retrievalbased mechanism which pops up the user's comprehension with the transformer's power and the external, knowledge-rich textual evidence during inference. By this, the user gets the help of contextual support that can dynamically change, thus the user can retrieve the scientific information that is relevant for more accurate classification of the complex structures. RAG's presence thus enhances interpretability and stability of performance.

4 Results and Discussion

In this section, we present the key graphical results from our experiments on the shape classification model. We evaluate performance using training curves and confusion matrices on the test set. The training curves present plots of loss, accuracy, macro F1-score, learning rate, train-validation loss difference, and the overfitting indicator, the latter defined as the difference in training and validation accuracy. Confusion matrices are normalized by row and color-coded to emphasize densities of predictions.

In each model, EfficientNet was applied for encoding SEM/TEM images and a transformer-based encoder for encoding text with cross-modal attention mechanisms. The dataset consists of 3,501 labeled data points from the models divided into training, validation and testing datasets. All models were evaluated on a held-out test set of 676 samples [17].

4.1 Overall Performance Comparison

Table 1 summarizes the overall performance metrics across three architectures. The model developed based on RAG achieved the best accuracy and Macro-F1 because of the enhanced retrieval capabilities.

Table 1: Comparison of Different Models on Evaluation Metrics

Model	**Accuracy**	**Macro-F1**	**Precision**	**Recall**
PubMedBERT	0.8512	0.6831	0.7124	0.6648
RoBERTa (Baseline)	0.8697	0.7215	0.7482	0.7043
RoBERTa + RAG	**0.9202**	**0.8288**	**0.7716**	**0.7318**

4.2 Class Wise Analysis

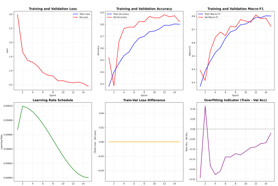
As shown by the class-wise F1-score comparison in Table 2, there is a significant enhancement in recognizing the minority class, especially the class "triangle".

The training curves for all three experimental runs are shown in Figs. 3a–3c. These figures elucidate model performance across training epochs, thereby illuminating convergence behavior, generalization capacity, and potential overfitting phenomena.

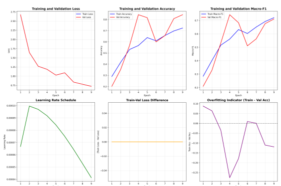
Figures 4a–4c depict the confusion matrices on the test sets for the three runs. By normalizing the matrices, it enables the user to see how many correct predicted

Table 2: Per-class F1-Scores Across Models

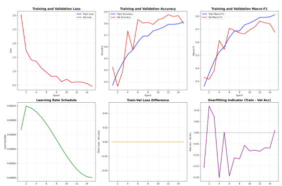
Class	**PubMedBERT**	**RoBERTa**	**RoBERTa + RAG**
Cube	0.842	**0.861**	0.853
Rod	0.764	0.781	**0.774**
Sphere	0.897	**0.903**	0.895
Triangle	0.338	0.381	**0.650**



(a) PubMedBERT: (i) loss, (ii) accuracy, (iii) macro F1, (iv) learning rate, (v) loss gap, (vi) overfitting indicator.



(b) RoBERTa: Same plots as Fig 3a. Notable fluctuations in accuracy and macro F1, suggesting hyperparameter sensitivity.



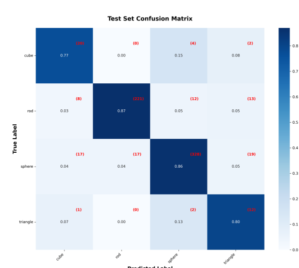
(c) RoBERTa+RAG: Same plots as Fig 3a. High accuracy with improvements in macro F1-score.

Fig. 3: Training and validation curves for PubMedBERT, RoBERTa, and RoBERTa+RAG models.

labels each class received based on true labels being predicted. The darker an area is on these matrices, the more of that true label has been attributed to that predicted label. Hence, these visualizations demonstrate the model's accuracy across runs, with average test accuracies inferred from the matrices range from approx. 0.75 to 0.85.

(a) PubMedBERT: High accuracy for 'rod' (0.94) and 'sphere' (0.86); minor 'cube'.

(b) RoBERTa: Strong diagonal; 'rod' (0.92), 'triangle' (0.73); fewer errors.



(c) RoBERTa+RAG: Darker Diagonal; 'sphere' (0.87) with 'cube' and 'triangle'.

Fig. 4: Test set confusion matrices across models.

Table 3: **Contributions Towards Addressing Identified Research Gaps**

Research Gap	**Our Contribution**	**Addressed**
Absence of standardized SEM/TEM metrics [6] [9] [13]	Standardized preprocessing, for example, ImageNet normalization. This allows for cross-dataset model training and evaluation.	✓
Lack and imbalance in annotated nanoparticle data [8] [15] [16]	RAG-enhanced RoBERTa extends training on external knowledge, reducing the need to annotate manually.	✓
Poor adaptation of LLMs/VLMs to microscopy [2] [3] [7]	Fine-tuned PubMedBERT and RoBERTa on scientific text for nanomaterial morphology classification.	✓
Weak multimodal fusion for visual-text alignment [1] [14] [17]	Novel cross-modal attention mechanism aligns visual features with text embeddings.	✓
Lacking fusion of complementary data sources [1] [2] [7] [13]	Merges high-resolution SEM/TEM images with scientific annotations, improving the accuracy of classification.	✓

5 Limitations of the Study

Despite its promising performance, the proposed multimodal framework has certain limitations. First, the dataset is derived primarily from literature-mined SEM/TEM images, which may introduce publication bias and limit generalization to proprietary or in-situ microscopy data. Second, the reliance on high-quality textual annotations restricts applicability in scenarios where metadata is incomplete or noisy. Third, retrieval-augmented generation increases computational overhead during inference, which may pose challenges for real-time deployment. Finally, the current study focuses on morphological classification and does not yet extend to fine-grained physicochemical property prediction.

6 Conclusion

In this work, a deep learning system has been developed for the automated characterization of nanomaterials by integrating high-resolution SEM/TEM images and specific textual information from scientific literature. Experimental evaluations showed that the Retrieval-Augmented RoBERTa variant achieved the highest accuracy of 92.02% with a Macro-F1 score of 0.8288. The notable 65% improvement in the F1-score for the triangle class emphasizes the model's better generalization and the importance of retrieval-based multimodal support for balanced performance across all categories.[13] [14]. The findings of this research could have an impact on future research to predict certain physicochemical properties of materials such as crystallinity, bandgap and surface reactivity. Self-supervised and few-shot meta-learning strategies will also improve performance with limited labeled data.[16] [3] Overall, this study lays a solid base for intelligent, multimodal, and interpretable nanomaterial analysis.

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