Graph Representation Learning for Predicting Material Properties from Microstructure Images

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I. A B S T R A C T

Predicting the processing parameters and chemical composition from the microstructure morphology is a key challenge in materials engineering. Accurate inverse mapping from morphology to material processing history can accelerate the design of advanced materials with tailored properties. While physics-based methods like phase-field modeling can simulate the evolution of microstructures under various conditions, they are often computationally expensive and not suitable for inferring the input parameters from observed morphologies. To address this inverse problem efficiently, we propose a graph neural network-based framework that learns microstructure-relationships from microstructure images using GraphSAGE convolution layers. Our case study involves a dataset generated from spinodal decomposition simulations of Fe–Cr–Co alloys, where each microstructure image is converted into a graph representation that captures pixel intensity-based neighborhood relationships. The input graphs encode local elemental distribution and feature connectivity, while the target labels include processing temperature and initial alloy composition. We utilize GraphSAGE architecture to perform regression on these graph representations, allowing the model to capture both local and global morphological patterns effectively.

II. Introduction

The development of materials with tailored properties is often limited by the high costs and extensive time associated with traditional trial-and-error methods. While advancements in multi-scale simulations and modeling have alleviated some challenges, they remain computationally intensive and fail to fully exploit the available experimental and simulated data [1]. To address these inefficiencies, we propose an integrated data-driven framework that aims to uncover complex relationships between processing parameters, microstructure, and material properties, collectively referred to as process-structure-property (PSP) linkages [2].

Recent advancements in data science and machine learning have opened promising new directions for addressing these challenges [3]. Traditional methods like Convolutional Neural Networks (CNNs) have shown success in analyzing structured, grid-based data such as images [4] [5] [6] [7]. However, their application in materials science is often constrained by the irregularity and complexity of microstructure data, making it difficult to effectively capture relationships between microstructural features and their spatial and compositional dependencies.

To overcome these limitations, we propose the use of graph-based representations as an efficient and extensible solution for modeling microstructure-sensitive systems [8]. By representing microstructures as labeled, weighted, undirected graphs, this approach will capture the intricate spatial and compositional relationships that are critical to understanding material behavior [9]. In our proposed framework, nodes will correspond to individual pixels, and edges will represent spatial interactions or compositional gradients, allowing for a detailed characterization of microstructures. To further enhance the utility of graph-based representations, we propose leveraging Graph Neural Networks (GNNs) to learn complex, non-linear dependencies from graph-structured data [10]. Unlike CNNs, which rely on structured grids and often struggle with irregularities in data, GNNs are inherently designed to handle the flexible and heterogeneous nature of graph-based inputs [11]. This makes GNNs particularly advantageous for modeling microstructure data, where spatial relationships and compositional gradients are irregular and not easily represented in a grid format. Our proposed framework will utilize GraphSAGE, a state-of-the-art GNN architecture, to predict key material properties—such as temperature, time, and chemical composition—from microstructure-derived graph representations. Node attributes will be defined by scaled pixel values, and edges will capture meaningful spatial relationships within the microstructure.

In this project, we propose to explore the application of Graph Neural Networks (GNNs) for modeling the relationships between microstructure and material properties, such as temperature, and elemental composition. The inherent flexibility of GNNs will allow them to process and learn from the complex microstructural data often encountered in materials

science, including data obtained from electron microscopy or simulations [12]. Through this proposal, we will develop a scalable and interpretable framework for material design that reduces computational and experimental costs traditionally associated with materials science [13].

A. Mapping Courses to Project Preparation

Throughout my Master's journey, I have taken a range of courses that have provided the foundational knowledge and technical skills necessary to develop this project. Courses such as **Introduction to Data Science**,**Machine Learning**, **Neural Networks**, **Natural Language Processing**, **Advanced Algorithms**, and **Databases** have been particularly instrumental.

- **Machine Learning & Neural Networks:** These courses equipped me with an understanding of various deep learning techniques, including Graph Neural Networks (GNNs), which are central to this project. The knowledge gained in feature extraction, model optimization, and performance evaluation directly supports the development of the GraphSAGE-based predictive model proposed in this work.
- **Advanced Algorithms:** This course helped in designing efficient data structures and optimization strategies, which are essential for graph-based learning and large-scale data processing in this project.
- **Natural Language Processing (NLP):** While NLP primarily deals with textual data, it provided experience in working with complex structured data and deep learning frameworks, which translates well to graph-based learning.
- **Databases:** The skills learned in managing structured and unstructured data are crucial for handling the GraphML dataset, ensuring efficient data storage, retrieval, and preprocessing.
- **Other Data Science & CS Courses:** Additional coursework in data science, statistical modeling, and AI has contributed to my ability to develop, train, and validate machine learning models for real-world applications.

B. Mapping Project Scope and Deliverables to MS in CS PLOs

This project aligns with the **Program Learning Outcomes (PLOs)** for the MS in Computer Science, as it demonstrates proficiency in the following areas:

- **Applying Theoretical Knowledge to Real-World Problems**
  - The project bridges graph theory, deep learning, and material science, demonstrating the ability to apply computational techniques to interdisciplinary challenges.
  - It showcases the use of advanced machine learning models (GraphSAGE) for processing complex microstructure data.
- **Designing and Developing Efficient Algorithms**
  - The project involves implementing graph-based data structures and designing optimized learning pipelines for material property prediction.
  - It utilizes efficient algorithmic approaches to manage and process large-scale datasets, addressing computational complexity challenges.

III. Related Work

The integration of graph-based models and deep learning [14] [15] [16] [17]techniques has shown significant potential in advancing material property predictions from microstructure images. This section provides an overview of the key studies that have informed and inspired our proposed methodology.

A. Graph-Based Approaches in Microstructure Analysis

Du et al. (2018) introduced a graph-based surrogate model to map microstructure characteristics to material performance metrics [8]. Their work highlighted the efficiency of graph representations in capturing domain-specific features such as connectivity, centrality, and domain sizes. They demonstrated how probabilistic optimization algorithms could be linked with graph models to perform global searches efficiently, providing a robust framework for microstructure-performance mapping.

Storm et al. (2024) explored the application of GNNs to microstructure-sensitive systems, emphasizing the scalability of these models for large-scale material datasets [11]. Their research demonstrated the efficacy of message-passing mechanisms in capturing hierarchical material features, paving the way for GNN-based surrogate models in computational material design.

Miao et al. (2023) proposed a Physics-Informed Neural Network (PINN) with Graph Embedding (GPINN), enhancing the performance of PINNs by incorporating topological features from graph-structured data [18]. This approach bridges the gap between data-driven models and physics-based simulations, significantly improving the accuracy of predictions in complex material systems.

Xiang et al. (2024) presented a novel approach combining Partial Differential Equations (PDEs) with Physics-Informed GNNs to model PSP linkages more effectively [1]. Their framework integrates physical laws directly into the learning process, allowing for robust predictions even with limited experimental data.

Kazemzadeh et al. (2022) demonstrated the use of deep learning models for predicting processing history from microstructure images, focusing on time and temperature parameters [4]. Their CNN-based framework achieved promising results but was limited by its inability to capture irregular spatial dependencies, a challenge that GNNs are well-suited to address.

Louis et al. (2020) introduced a novel graph neural network architecture, GATGNN, designed to improve materials property prediction by incorporating global attention mechanisms [19]. The GATGNN framework integrates both Graph-Attention Layers (AGAT) and a Global Attention Layer to enhance the learning of local and global structural relationships within material graphs.

Crystal Graph Convolutional Neural Networks (CGCNN) by Tian Xie and Jeffrey C. Grossman (2018) [20] introduces a generalized framework for predicting material properties directly from crystal structures. Unlike traditional machine learning models that rely on handcrafted features, CGCNN learns representations from the atomic connections within crystals. This approach achieves high accuracy in predicting properties such as formation energy, band gap, and elastic moduli.

METHODS

B. Model Material and Database Generation:

The model material in this study is FeCrCo ternary alloy. FeCrCo alloys experience phase separation, i.e., spinodal decomposition, at temperatures between 500 C to 700 C. The dataset used in this work was generated using a phase-field simulation of spinodal decomposition in FeCrCo ternary alloys. The simulation models the evolution of microstructure under varying thermal and chemical conditions using the Cahn–Hilliard equations [21], where Cr and Co concentrations were treated as conserved variables. The total free energy functional includes contributions from chemical free energy, elastic strain energy, and magnetic interactions. The simulation parameters such as temperature, Cr, and Co compositions were varied systematically to generate a comprehensive database of microstructure images and corresponding processing conditions. The simulation framework and governing equations were adopted from a prior study [22] and we refer the interested readers to [4] for more details about the phase field model. In database generation we explored the chemistry space between 0.05 to 0.9, with 0.05 grid, for both Cr and Co and for temperature we studied the range of 853 K to 963 K, with 10 K grid. The dataset was generated using a Simplex-Lattice mixture design to cover the ternary Fe–Cr–Co composition space, ensuring that the sum of concentrations equals one. All simulations ran for 100 hr heat treatment. After simulations we end up with 389 morphologies that had spinodal decomposition. The result of each simulation was a 2D microstructure image representing the Fe concentration field, which reflects the morphology resulting from spinodal decomposition under the specified conditions. Each image in the dataset is thus associated with a unique set of processing parameters (temperature, Cr composition, Co composition), which we treat as target variables for supervised learning.

C. Graph Construction from Materials Elemental Morphology

1) **Image Preprocessing**: For the proposed model, we used Fe-based morphologies. Each microstructure image was first converted to grayscale, where pixel intensities ranged from 0 to 255. These grayscale values represent the relative Fe concentration fields output from the phase-field simulations. The grayscale image was then resized to 224 × 224 pixels to ensure consistent input dimensions across all samples. This standardization is crucial for the generation and training of downstream graphs [23]. The graph construction process plays a critical role in determining the effectiveness of a Graph Neural Network (GNN) model, as it defines how raw data are structured into nodes and edges suitable for graph-based learning.
2) **Node Feature Representation via Fe Concentration Scaling**:
To convert grayscale pixel intensities into physically meaningful values, we applied a linear scaling transformation [24] that maps the original pixel intensity range $[0, 255]$ to the actual Fe concentration range $[\mathrm{c}^{\mathrm{Fe}}_{\min}, \mathrm{c}^{\mathrm{Fe}}_{\max}]$. As a result, each pixel in the image corresponds to a localized Fe concentration value.
When converting images to graphs, each pixel is treated as a node, and its corresponding scaled Fe concentration value is assigned as the node feature as shown in Table I. This ensures that the graph representation retains quantitative information about the underlying microstructure morphology. For a pixel located at position (i, j), the node feature $x_{ij} \in \mathbb{R}$ is computed as:

$$x_{ij} = a \cdot \text{image}[i, j] + b$$

where

$$a = \frac{M_0 - m_0}{M_1 - m_1} \quad \text{and} \quad b = m_0 - a \cdot m_1$$

3) **Edge Formation:** Edges are created between each pixel and its immediate neighbors—including right, bottom, and diagonal neighbors—encoding the local spatial structure in the image. We consider connectivity in a row-major, column-major, and diagonal manner to comprehensively capture local topology. The edge weights are computed as the absolute difference in scaled pixel intensity between the connected nodes. For example, the weight of an edge between pixels at (i, j) and $(i, j+1)$ is given by:

$$w_{(i,j)\to(i,j+1)} = |\text{scaled\_image}[i, j] - \text{scaled\_image}[i, j+1]|$$

This simple yet effective method emphasizes contrast boundaries in the image, allowing the Graph Neural Network (GNN) to learn from local variations in microstructure morphology.
In our graph construction from elemental morphologies, we use undirected edges only, i.e., if a connection exists from node A to node B, the reverse connection from B to A is also present [25]. We assume symmetrical weights for these edges, meaning:

$$w_{A\to B} = w_{B\to A}$$

This design choice ensures that information flows bidirectionally between connected pixels, enhancing the model's ability to capture local geometric and intensity-based patterns.

TABLE I
DESCRIPTION OF VARIABLES USED FOR INTENSITY SCALING.

Variable	Value	Description
m_0	0.1	minimum Fe concentration
M_0	0.46	maximum Fe concentration
m_1	0	minimum pixel value in the image
M_1	255	maximum pixel value in the image

4) **Graph Labels:** Each graph is labeled with target values representing physical or material properties of interest. In this study, each graph is associated with a three-dimensional target vector [T,Cr,Co], corresponding to temperature and concentrations of chromium (Cr) and cobalt (Co), respectively. These labels are used for supervised regression tasks during model training.
5) **Graph Format and Storage:** We propose transforming microstructure images into labeled, weighted, undirected graphs $G = (V, E, W, L)$ as shown in the fig 1 Constructed graphs are stored in the GraphML format to preserve node features, edge indices, and graph-level labels. This format allows seamless loading and preprocessing using PyTorch Geometric and igraph, ensuring consistency and scalability across the dataset.

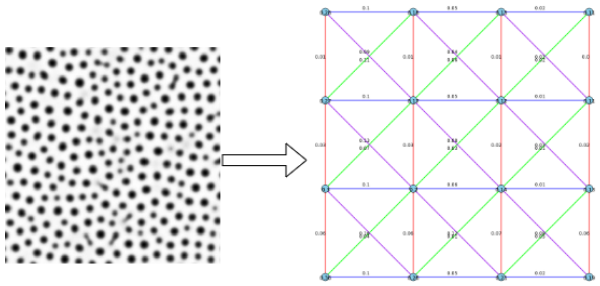

Fig. 1. Graph Construction

D. Deep Learning Methodology

In this work, we develop a graph-based deep learning framework to perform inverse mapping from microstructure morphology to processing parameters. Given the mixed nature of our dataset — consisting of both image-derived graph data and scalar numerical features — a model capable of handling structured and unstructured input is essential [26]. We use a Graph Neural Network (GNN), specifically the GraphSAGE architecture, to extract hierarchical features from graph-structured representations of microstructure images. Graph Neural Networks (GNN) are classes of deep learning models specifically designed to work with data that is best represented as graphs rather than grids. GNNs are especially well-suited for applications where relationships between entities — such as spatial, topological, or chemical interactions — are irregular, non-Euclidean, or cannot be captured effectively using traditional grid-based approaches like convolutional neural networks (CNNs). GNNs, like other deep learning architectures, consist of input, hidden, and output layers. However, the key difference lies in how they propagate information: instead of using convolution over pixels, GNNs perform neighborhood aggregation where each node in a graph updates its representation by aggregating features from its neighboring nodes.

One of the widely adopted GNN architectures is GraphSAGE [27] [28] 29 [30], which operates through a series of message-passing layers. In each layer, a node samples and aggregates features from its neighbors using predefined aggregation functions (such as mean, sum, or LSTM-based aggregators). This process allows the network to capture local context and long-range dependencies simultaneously. The graph embedding generated by these layers serves as a high-level summary of the entire structure and can be used for downstream tasks such as classification or regression. In our work, the grayscale microstructure images were converted into graphs where each pixel or region represents a node, and edges were constructed based on spatial adjacency and similarity of intensity (Fe composition). These graphs are input to the GNN, which learns morphological representations directly from the topology of the microstructure, rather than relying on fixed spatial filters as in CNNs. This flexibility makes GNNs more suitable for capturing the complex, non-grid-based morphology common in materials science datasets.

Like other neural networks, Graph Neural Networks (GNNs) are trained using a loss function and backpropagation to update model parameters. In this study, we adopted a deep GraphSAGE architecture composed of eight message-passing layers, each using mean aggregation to capture local and global structural features from the microstructure graphs. After the graph-level embedding is obtained via global mean pooling, it is passed through a series of five fully-connected layers for final regression. All hidden layers utilize the ReLU activation function to introduce nonlinearity. Figure 2 shows the schematic of the proposed framework. The model was trained to minimize the mean absolute error (L1 loss) between predicted and true processing parameters. Weight initialization was applied to both the GraphSAGE layers (Xavier initialization) and fully-connected layers (He initialization) to ensure stable convergence during training. Optimization was performed using the Adam optimizer with a fixed learning rate. Specific architectural and training hyperparameters are summarized in Table II.

DATASET AND EXPERIMENTAL SETUP

To establish a controlled and focused experimental framework, we propose initially selecting GraphML files representing microstructure images processed for 100 hours. This approach will simplify the problem space by fixing the

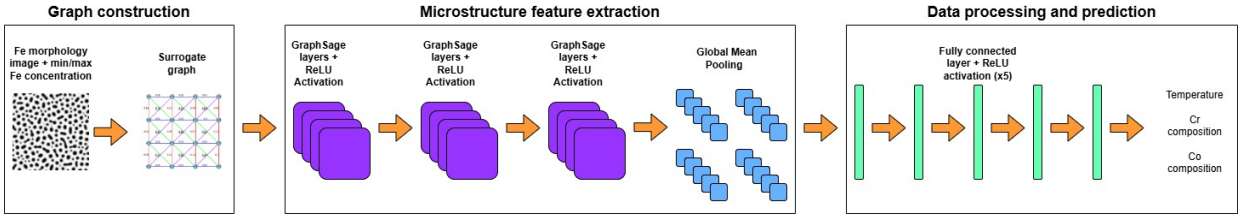

Fig. 2. GraphSAGE Architecture for Microstructure Regression

processing time as a constant parameter, thereby reducing variability and enabling a more precise analysis of process-structure-property (PSP) linkages—specifically, the relationships between microstructure, temperature, and chemical composition. This initial dataset will provide a foundational basis for evaluating the feasibility and effectiveness of our proposed framework. However, to enhance the generalizability and robustness of our model, we plan to expand the dataset in subsequent iterations by incorporating additional processing conditions, such as varying time and temperature parameters.

TABLE II
PARAMETERS SELECTED FOR GRAPHSAGE MODEL SPECIFICATION, COMPILATION, AND TRAINING.

Parameter	Selected Value or Option
Model Specification	
Number of GraphSAGE Layers	8
Aggregation Function	Mean
Hidden Channels	128
Output Dimension	3 (Cr composition, Co composition, Temperature)
Activation Function	ReLU
Initialization	Xavier for GraphSAGE layers, He for fully connected layers
Compilation	
Loss Function	Mean Absolute Error (MAE)
Optimizer	Adam
Learning Rate	0.001
Batch Size	32
Gradient Clipping	Max norm = 5.0
Training Setup	
Epochs	1000
Training Data Split	80%
Testing Data Split	20%
Dataset Representation	Graphs from 100-hour dataset (time removed)

RESULTS AND DISCUSSION

E. Model Learning Behavior

The learning curve and GraphSage pipeline in Figure 3 and Figure 4 illustrates the training and test loss trajectories of the proposed GraphSAGE model over 1000 epochs. Both the training and test loss decrease rapidly during the initial phase (approximately the first 50 epochs), indicating that the model effectively learns from the microstructure graph data early in the training process. After around 200 epochs, the losses begin to stabilize, with the training loss continuing to gradually decline while the test loss remains relatively constant. The test loss consistently remains slightly higher than the training loss, which is expected and suggests that the model generalizes well without significant overfitting. While minor fluctuations are observed in the test loss, they are relatively small and likely reflect variability in the test data rather than model instability. Overall, the learning curve indicates that the GraphSAGE model achieves a good balance between learning and generalization. Given the early convergence behavior, incorporating early stopping could reduce training time without sacrificing performance.

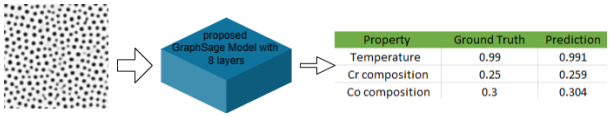

Fig. 3. GNN-based prediction pipeline using an 8-layer GraphSAGE model

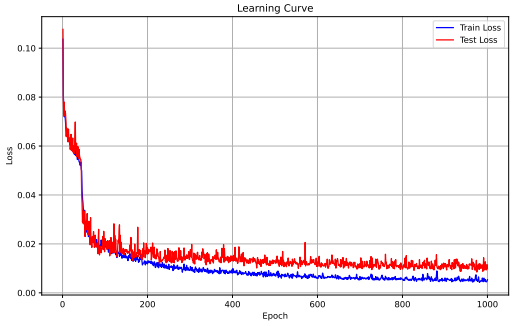

Fig. 4. Gnn learning curve

F. GNN Performance on Temperature and Composition Prediction:

1) **Chromium (Cr) Prediction:** The parity plot as shown in fig : 5 for chromium (Cr) demonstrates a high level of agreement between the predicted and true values, with an R^2 score of 0.977 and a mean squared error (MSE) of 1.04×10^{-4}. The data points align closely along the diagonal line representing perfect prediction, indicating that the model effectively captures the underlying relationship between microstructural features and Cr concentration. This level of accuracy is critical for alloy design tasks where small variations in elemental composition can significantly influence material properties.

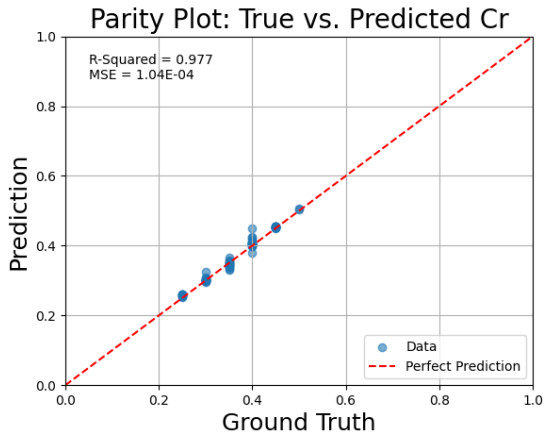

Fig. 5. Parity Plot Chromium

2) **Cobalt (Co) Prediction:** The model's performance on cobalt (Co) prediction also shows strong accuracy as shown in fig : 6, with an R^2 of 0.975 and an MSE of 5.89×10^{-4}. The parity plot reveals a tight clustering of predictions around the ideal diagonal, suggesting the model's robustness in learning Co-related features from the microstructure graph. Accurate estimation of Co content is essential in tuning phase stability and mechanical performance in multi-component alloys, emphasizing the utility of graph-based learning for composition-property mapping.

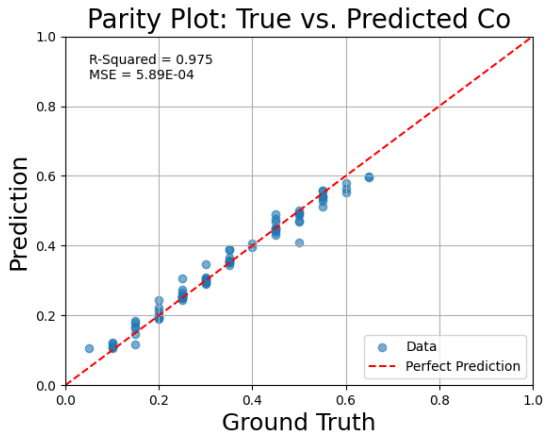

Fig. 6. Parity Plot Cobalt

3) **Temperature Prediction:** The parity plot for temperature prediction illustrates good predictive performance in the fig: 7, with an R^2 of 0.942 and an MSE of 6.13×10^{-5}. While the values span a narrower range compared to Cr and Co, the predictions remain well-aligned with the ground truth, with minimal deviation from the perfect prediction line. This suggests the model's ability to infer thermal processing conditions from static microstructural information, supporting its application in inverse process modeling and microstructure-informed parameter retrieval.

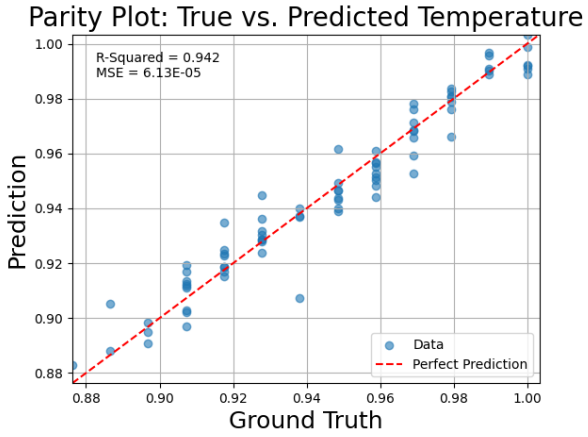

Fig. 7. Parity Plot Temperature

G. Comparison of GNN and CNN Performance:

A detailed comparison between the proposed GraphSAGE-based Graph Neural Network (GNN) and a state-of-the-art EfficientNet-based Convolutional Neural Network (CNN) [22] in fig: 8 underscores the superior performance and broader applicability of GNNs for microstructure-informed property prediction. While the CNN achieves slightly higher accuracy in predicting cobalt (Co) composition with an R^2 of 0.9962 compared to 0.975 for the GNN, the GNN outperforms the CNN on both chromium (Cr) composition ($R^2 = 0.977$ vs. 0.955) and temperature prediction ($R^2 = 0.942$ vs. 0.9319). This demonstrates the GNN's stronger generalization capability and its robustness across different types of physical parameters.

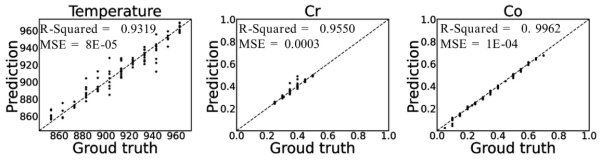

Fig. 8. Comparison Analysis with CNN Model

More importantly, GNNs provide a structural advantage by modeling the microstructure as a graph, where each pixel is treated as a node and edge connections encode local spatial or chemical relationships. This enables the GNN to directly exploit topological and morphological cues that are often lost or diluted in grid-based CNN representations. By capturing these intrinsic microstructural interactions, the GNN offers a more physically meaningful and interpretable learning framework. Such structured representations are particularly powerful in materials science, where morphology, phase boundaries, and compositional gradients significantly influence the processing–structure–property relationship.

Overall, while both models are effective, the GNN architecture demonstrates a higher degree of flexibility, physical

relevance, and interpretability, making it a more suitable choice for inverse materials design and high-fidelity property inference from microstructural data.

Conclusion

In this work, we presented a graph-based deep learning framework utilizing a GraphSAGE architecture to predict processing parameters—namely chromium (Cr) and cobalt (Co) compositions, as well as temperature—directly from microstructure images. By transforming grayscale microstructures into graph representations, the model effectively captured local morphological and compositional features using node-wise relationships and edge-based interactions. The proposed GNN model achieved high predictive performance across all targets, with parity plots showing strong agreement between predicted and ground truth values and R^2 scores consistently exceeding 0.94.

Compared to a state-of-the-art CNN model (EfficientNet), our GraphSAGE-based approach demonstrated comparable or superior performance, particularly in predicting Cr and temperature. More importantly, the GNN framework offers greater interpretability and physical relevance by directly modeling pixel connectivity and topological relationships—an advantage especially critical in microstructure-informed inverse design and materials discovery.

Overall, this study highlights the promise of Graph Neural Networks in materials informatics, showcasing their ability to generalize well across diverse properties while leveraging graph-structured inputs derived from image-based morphology. Future work will explore the integration of multimodal data (e.g., phase fields, strain maps) and the incorporation of uncertainty quantification to further enhance the model's reliability and applicability in real-world materials design pipelines.

References

[1] Z. Xiang, W. Peng, W. Yao, X. Liu, and X. Zhang, "Solving spatiotemporal partial differential equations with physics-informed graph neural network," *Preprint or Journal Name (if known)*, 2023, add specific journal, volume, issue, and page numbers if published. Update with DOI or URL if available.

[2] A. Thomas, A. R. Durmaz, M. Alam, P. Gumbsch, H. Sack, and C. Eberl, "Materials fatigue prediction using graph neural networks on microstructure representations," *Scientific Reports*, vol. 13, p. 12562, 2023.

[3] J. Schmidt, M. R. Marques, S. Botti, and M. A. Marques, "Recent advances and applications of machine learning in solid-state materials science," *npj Computational Materials*, vol. 5, p. 83, 2019. [Online]. Available: https://doi.org/10.1038/s41524-019-0221-0

[4] A. A. Kazemzadeh Farizhandi and M. Mamivand, "Processing time, temperature, and initial chemical composition prediction from materials microstructure by deep network for multiple inputs and fused data," *Materials & Design*, vol. 223, p. 110799, 2022. [Online]. Available: https://doi.org/10.1016/j.matdes.2022.110799

[5] Y. Chen, S. Duffner, A. Stoian, J.-Y. Dufour, and A. Baskurt, "Deep and low-level feature based attribute learning for person re-identification," *Image and Vision Computing*, vol. 80, pp. 1–9, 2018. [Online]. Available: https://doi.org/10.1016/j.imavis.2018.09.006

[6] G. E. Hinton, "To recognize shapes, first learn to generate images," in *Progress in Brain Research*. Elsevier, 2007, vol. 165, pp. 535–547. [Online]. Available: https://doi.org/10.1016/S0079-6123(06)65034-6

[7] Y. LeCun, Y. Bengio, and G. Hinton, "Deep learning," *Nature*, vol. 521, no. 7553, pp. 436–444, 2015. [Online]. Available: https://doi.org/10.1038/nature14539

[8] P. Du, A. Zebrowski, J. Zola, B. Ganapathysubramanian, and O. Wodo, "Microstructure design using graphs."

[9] D. Joyner, M. V. Nguyen, and D. Phillips, *Algorithmic Graph Theory and Sage*, version 0.8-r1991 ed. Self-published, 2013. [Online]. Available: http://code.google.com/p/graphbook/

[10] W. L. Hamilton, *Graph Representation Learning*, ser. Synthesis Lectures on Artificial Intelligence and Machine Learning. Morgan & Claypool Publishers, 2020, vol. 14, no. 3, pre-publication draft, unedited version released with permission. Relevant copyrights held by the author and publisher.

[11] J. Storm, I. B. C. M. Rocha, and F. P. van der Meer, "A microstructure-based graph neural network for accelerating multiscale simulations," *Delft University of Technology, Department of Civil Engineering and Geosciences*, 2023, preprint or update with publication details if available.

[12] R. Pollice, G. d. P. Gomes, M. Aldeghi, R. J. Hickman, M. Krenn, C. Lavigne, M. Lindner-D'Addario, A. K. Nigam, C. T. Ser, Z. Yao, and A. Aspuru-Guzik, "Data-driven strategies for accelerated materials design," *Accounts of Chemical Research*, vol. 54, no. 4, pp. 849–860, 2021.

[13] K. Choudhary, B. DeCost, C. Chen, A. Jain, F. Tavazza, R. Cohn, C. W. Park, A. Choudhary, A. Agrawal, S. J. L. Billinge, E. Holm, S. P. Ong, and C. Wolverton, "Recent advances and applications of deep learning methods in materials science," *npj Computational Materials*, vol. 8, p. 59, 2022, published: 05 April 2022. [Online]. Available: https://www.nature.com/articles/s41524-022-00735-x

[14] J. E. Gubernatis and T. Lookman, "Machine learning in materials design and discovery: Examples from the present and suggestions for the future," *Physical Review Materials*, vol. 2, no. 12, p. 120301, 2018. [Online]. Available: https://doi.org/10.1103/PhysRevMaterials.2.120301

[15] D. Jha, L. Ward, A. Paul, W.-k. Liao, A. Choudhary, C. Wolverton, and A. Agrawal, "Elemnet: Deep learning the chemistry of materials from only elemental composition," *Scientific Reports*, vol. 8, no. 1, p. 17593, 2018. [Online]. Available: https://doi.org/10.1038/s41598-018-35934-y

[16] D. Xue, D. Xue, R. Yuan, Y. Zhou, P. V. Balachandran, X. Ding, J. Sun, and T. Lookman, "An informatics approach to transformation temperatures of niti-based shape memory alloys," *Acta Materialia*, vol. 125, pp. 532–541, 2016. [Online]. Available: https://doi.org/10.1016/j.actamat.2016.12.009

[17] B. Meredig, E. Antono, C. Church, M. Hutchinson, J. Ling, S. Paradiso, B. Blaiszik, I. Foster, B. Gibbons, J. Hattrick-Simpers, A. Mehta, and L. Ward, "Can machine learning identify the next high-temperature superconductor? examining extrapolation performance for materials discovery," *Molecular Systems Design & Engineering*, vol. 3, no. 5, pp. 819–825, 2018. [Online]. Available: https://doi.org/10.1039/C8ME00012C

[18] Y. Miao and H. Li, "Gpinn: Physics-informed neural network with graph embedding," *arXiv preprint arXiv:2306.09792*, 2023. [Online]. Available: https://arxiv.org/abs/2306.09792

[19] S.-Y. Louis, Y. Zhao, A. Nasiri, X. Wang, Y. Song, F. Liu, and J. Hu, "Graph convolutional neural networks with global attention for improved materials property prediction," *Physical Chemistry Chemical Physics*, vol. 22, no. 32, pp. 18 141–18 148, 2020. [Online]. Available: https://doi.org/10.1039/d0cp01474e

[20] T. Xie and J. C. Grossman, "Crystal graph convolutional neural networks for an accurate and interpretable prediction of material properties," *Physical Review Letters*, vol. 120, no. 14, p. 145301, 2018. [Online]. Available: https://doi.org/10.1103/PhysRevLett.120.145301

[21] E. Moshkelgosha and M. Mamivand, "Concurrent modeling of martensitic transformation and crack growth in polycrystalline shape memory ceramics," *Engineering Fracture Mechanics*, vol. 241, p. 107403, 2021. [Online]. Available: https://doi.org/10.1016/j.engfracmech.2020.107403

[22] A. A. K. Farizhandi, O. Betancourt, and M. Mamivand, "Deep learning approach for chemistry and processing history prediction from materials microstructure," *Scientific Reports*, vol. 12, p. 4552, 2022. [Online]. Available: https://doi.org/10.1038/s41598-022-08484-7

[23] M. Dai, M. F. Demirel, Y. Liang, and J.-M. Hu, "Graph neural networks for an accurate and interpretable prediction of the properties of polycrystalline materials," *npj Computational Materials*, vol. 7, p. 103, 2021.

[24] M. Brockschmidt, "Gnn-film: Graph neural networks with feature-wise linear modulation," *arXiv preprint arXiv:1906.12192*, 2019. [Online]. Available: https://arxiv.org/abs/1906.12192

[25] Z. Wu, S. Pan, F. Chen, G. Long, C. Zhang, and S. Y. Philip, "A comprehensive survey on graph neural networks," *IEEE Transactions on Neural Networks and Learning Systems*, vol. 32, no. 1, pp. 4–24, 2021. [Online]. Available: https://ieeexplore.ieee.org/document/9046288

[26] Y. Wang, Y. Wang, J. Yang, and Z. Lin, "Dissecting the diffusion process in linear graph convolutional networks," *arXiv preprint arXiv:2102.10739*, 2021. [Online]. Available: https://arxiv.org/abs/2102.10739

[27] W. L. Hamilton, R. Ying, and J. Leskovec, "Inductive representation learning on large graphs," in *Advances in Neural Information Processing Systems*, vol. 30. Curran Associates, Inc., 2017, pp. 1024–1034.

[28] H. Hu, S. Wu, G. Cai, and N. Liu, "A physics-driven graphsage method for physical process simulations described by partial differential equations," *arXiv preprint arXiv:2403.08569*, 2024. [Online]. Available: https://arxiv.org/abs/2403.08569

[29] L. Gallo, V. Latora, and A. Pulvirenti, "Multisage: A multiplex embedding algorithm for inter-layer link prediction," *arXiv preprint arXiv:2206.13223*, 2022. [Online]. Available: https://arxiv.org/abs/2206.13223

[30] X. Wang and A. Vinel, "Benchmarking graph neural networks on link prediction," *arXiv preprint arXiv:2102.12557*, 2021. [Online]. Available: https://arxiv.org/abs/2102.12557