



# An image-based deep learning framework for predicting thermal conductivity of polymer composites with rotational data augmentation

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## ABSTRACT

Predicting the thermal conductivity of polymer-based composites with complex microstructures is critical for enhancing thermal flow in applications like electronics and electric vehicles. Traditional methods such as theoretical models and simulations often lack generalizability and are computationally expensive. This study proposes an efficient deep learning framework that predicts thermal conductivity from scanning electron microscopy (SEM) images. The model employs a multi-input convolutional neural network that combines 2D structural images, region-specific data, and latent features. A simulation dataset was created using random sequential adsorption to generate statistical volume elements (SVEs), which were analyzed through finite element thermal simulations. The resulting 3D models were converted into 2D images aligned along the heat-transfer direction and augmented via rotation. Regions of interest were annotated using bounding boxes and labeled as filler, inter-filler, or matrix. Global features were compressed into latent vectors using an autoencoder. The model was trained on 1,728 image-label pairs and achieved high prediction accuracy ( $R^2 = 0.9315$ , RMSE = 0.0664). These results confirm the model's effectiveness in capturing the complex relationship between composite microstructures and their thermal conductivity.

## 1. Introduction

The demand for composite materials with high thermal conductivities is rapidly increasing across a wide range of applications, including enhanced performance in electronic and semiconductor devices, safety in electric vehicle (EV) battery management systems, and thermal management in aerospace and renewable energy equipment. For example, EV batteries generate significant heat during operation, and failure to dissipate this heat effectively can lead to performance degradation and safety hazards. The development of thermally conductive composites that encapsulate these batteries is essential to improve the stability and efficiency of EV systems.

Particularly, polymer-based thermally conductive composites are actively studied owing to their design flexibility, high versatility, and cost-effectiveness [1,2]. Commonly used fillers include graphene nanoplatelets (GNPs) [3–5], carbon nanotubes (CNTs) [5–9], alumina ( $\text{Al}_2\text{O}_3$ ) [4,9,10], silicon carbide (SiC) [11], boron nitride (BN) [12,13], and highly conductive metal particles such as silver and copper [7,14,15]. The thermal conductivity of composites depends on both the intrinsic properties of the constituent materials and structural factors

such as the internal microstructure and filler distribution. Particularly, at smaller scales, the morphology (spherical, fibrous, or plate-like), loading content, and spatial distribution of these fillers significantly influence the thermal conductivity of composites. Therefore, accurate property prediction models must be developed. Microscale thermal conductivity refers to the heat transfer characteristics arising from the microstructure within composites. It is determined by factors such as the thermal pathways between fillers and the matrix, the size, shape, orientation, distribution of the fillers, and the interfacial thermal resistance.

This microscale thermal conductivity critically influences the macroscale thermal performance of the composite [16,17]. Notably, anisotropy, spatial distribution, and agglomeration of fillers can lead to localized heat concentration or obstruction.

Consequently, localized heat accumulation, known as hotspots, can occur within the composite, leading to thermal instability, performance degradation, and, in severe cases, fatigue failure [18]. Therefore, developing predictive models that accurately capture these microscale thermal conductivity characteristics is essential.

Conventional approaches for predicting the thermal conductivity of

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composites are primarily divided into theoretical and numerical-simulation-based models. Theoretical models are grounded in the effective medium theory (EMT), which assumes that a composite is a macroscopically homogeneous medium. For example, the Maxwell–Garnett model [19] is suitable for low-volume-fraction spherical fillers and the Hasselman model [20] improves on this by considering the filler size and interfacial thermal resistance (or Kapitza resistance). The Bruggeman model [21] assumes that all phases in the composite contribute equally, making it applicable even at higher filler loadings.

However, EMT-based models struggle to accurately reflect filler–filler interactions, clustering effects, and complex interfacial heat transfer mechanisms. This limits their predictive accuracy for composites with high filler content or irregular structure. To address these limitations, numerical simulation methods such as molecular dynamics (MD), the lattice Boltzmann method (LBM), and the finite element method (FEM) have been employed. For example, Yang et al. [22] conducted MD simulations to analyze the thermal and mechanical properties of an epoxy resin with carbon nanobuds. Kim et al. [6] calculated the interfacial resistance using MD and integrated it into a multiscale model to predict the thermal conductivity of polymer composites. Qu et al. [23] employed a modified LBM to incorporate porosity and interphase conductivity into aerogels, and Kan et al. [24] applied a D3Q15 LBM model to nanoporous structures generated using the quartet structure generation set. Ramani et al. [25] developed automated FEM models based on microstructural images, and Xu et al. [26] analyzed heat conduction in composites using randomly arranged fillers and automatic mesh generation.

Despite these advancements, numerical methods are still limited by their high computational costs and difficulty in generalizing structurally complex systems. To overcome these challenges, recent research has actively investigated approaches based on machine learning to predict material properties. For example, Liu et al. [27] used various multiscale features, such as the nanotube length, chirality, interfacial resistance, and dispersion, as inputs to predict the thermal conductivity of nanocomposites based on single-walled CNTs. Bhandari et al. [28] predicted the thermal conductivity of additively manufactured Fe- and Co-based alloys using composition and temperature as inputs. Liu et al. [29] applied physics-informed neural networks to predict the thermal conductivity of polyurethane phase change material composites by integrating physical equations with data-driven learning. Although these models allow for quantitative predictions based on numerical inputs, their ability to capture microstructural features, such as the filler shape, orientation, and spatial distribution, is limited. Because the thermal conductivity of a composite is highly sensitive to microstructural factors, a learning approach that directly uses structural images is required.

Accordingly, recent studies have applied deep-learning techniques, particularly convolutional neural networks (CNNs), to structural images. Liu et al. [30] extracted the filler orientation from image sets obtained from six faces of a 3D representative volume element by combining CNNs with a random forest regression model to predict thermal conductivity. Rong et al. [31] constructed sets of 2D cross-sectional images from 3D composite structures depending on the filler orientation. Ejaz et al. [32] predicted the thermal and electrical conductivities using CNNs trained on images obtained by the FEM simulation of aligned CNT composites. However, most of the above-mentioned studies assumed aligned filler structures or relied on sets of multiple images to incorporate 3D structural information. Such approaches increase the preprocessing complexity and limit the ability to generalize realistic randomly distributed filler structures.

To address these limitations, this paper proposes a framework that uses a multi-input CNN model. The proposed framework integrates a single 2D image of a composite with randomly distributed spherical fillers, its corresponding region of interest (ROI) information, and a latent vector as the model inputs to independently predict the thermal conductivity for each image. In this study, rotational transformations were applied to individual statistical volume elements (SVEs) [33] to

generate different structural images. Thus, a training dataset that reflects directional changes and structural variations was constructed using a limited number of base structures. The authors believe that this approach allows the model to learn effectively from various internal configurations and heat transfer pathways without repeatedly generating new SVEs or performing FEM simulations, which significantly reduces the data construction cost and simulation time.

## 2. Simulation-based data generation overview

The proposed approach aims to evaluate the feasibility of structure–property (thermal conductivity) mapping from micro-image representations under various structural configurations. The referenced data include the physical properties of the fillers and matrix that are typically used in composite materials, such as the thermal conductivity, filler size, volume fraction, and Kapitza resistance. These parameters significantly affect the formation of heat conduction pathways and the overall thermal performance of the composite by reflecting the interfacial interactions between the fillers and matrix. Particularly, the filler size and volume fraction influence the packing density and interfiller spacing, which, in turn, alter the effective thermal conductivity.

Based on these material properties, a simulation-driven dataset was constructed by generating SVEs, followed by thermal analysis and image-based processing. Notably, SVEs serve as representative unit cells that numerically model the microstructural configurations of composites, allowing for the effective representation of the internal architectures resulting from different filler–matrix combinations. As shown in Fig. 1, the database construction process comprises the following five steps: (1) SVE generation, (2) thermal analysis, (3) 2D image generation, (4) ROI generation, and (5) image-based feature extraction. Through this pipeline, a high-quality training dataset was established, wherein each image is associated with a thermal conductivity value obtained quantitatively using a simulation model. Subsequently, the resulting dataset was used as input to train the proposed CNN model. Each step is explained in detail in the following section.

## 3. SVE generation

To construct diverse microstructures with varying filler sizes and volume fractions, SVEs were generated as foundational structural units for the simulation. The process began by defining the target distribution of filler sizes and the desired volume fraction. A random sequential adsorption (RSA) [34,35] algorithm was implemented in MATLAB to determine the spatial coordinates of filler particles within a three-dimensional domain. The RSA algorithm places filler particles randomly within the simulation space and allows adsorption only in the event of no overlap with previously placed particles, thereby ensuring statistically realistic and physically nonoverlapping microstructures that mimic the random distribution of fillers in actual composites.

Each particle radius was randomly selected from a predefined range  $r_{\min} < r < r_{\max}$ , and a time increment  $\delta t$  was calculated based on the volume of the selected particle. If  $L$  denotes the side length of the domain, the time increment can be expressed as  $\delta t = 4\pi r^3/3L^3$  or alternatively as  $\delta t = 4\pi r^3/3N_A$ , where  $N_A$  is the number of particles in the system. This iterative process continued until the target volume fraction was reached, with each particle placed sequentially while maintaining nonoverlapping conditions. In this study, the domain was defined as a cube with a side length of 10  $\mu\text{m}$  (10  $\mu\text{m} \times 10 \mu\text{m} \times 10 \mu\text{m}$ ), corresponding to the size of each SVE used in the simulation.

Fig. 2 presents the filler size distribution measured from actual scanning electron microscopy (SEM) images, confirming that the generated filler distribution closely matched the average particle size and dispersion characteristics of real powder materials. Fig. 3 shows representative examples of generated SVE structures with varying volume fractions. The lower and upper bounds of the filler radius (1  $\mu\text{m}$  and 3  $\mu\text{m}$ , respectively) were determined based on the product specification

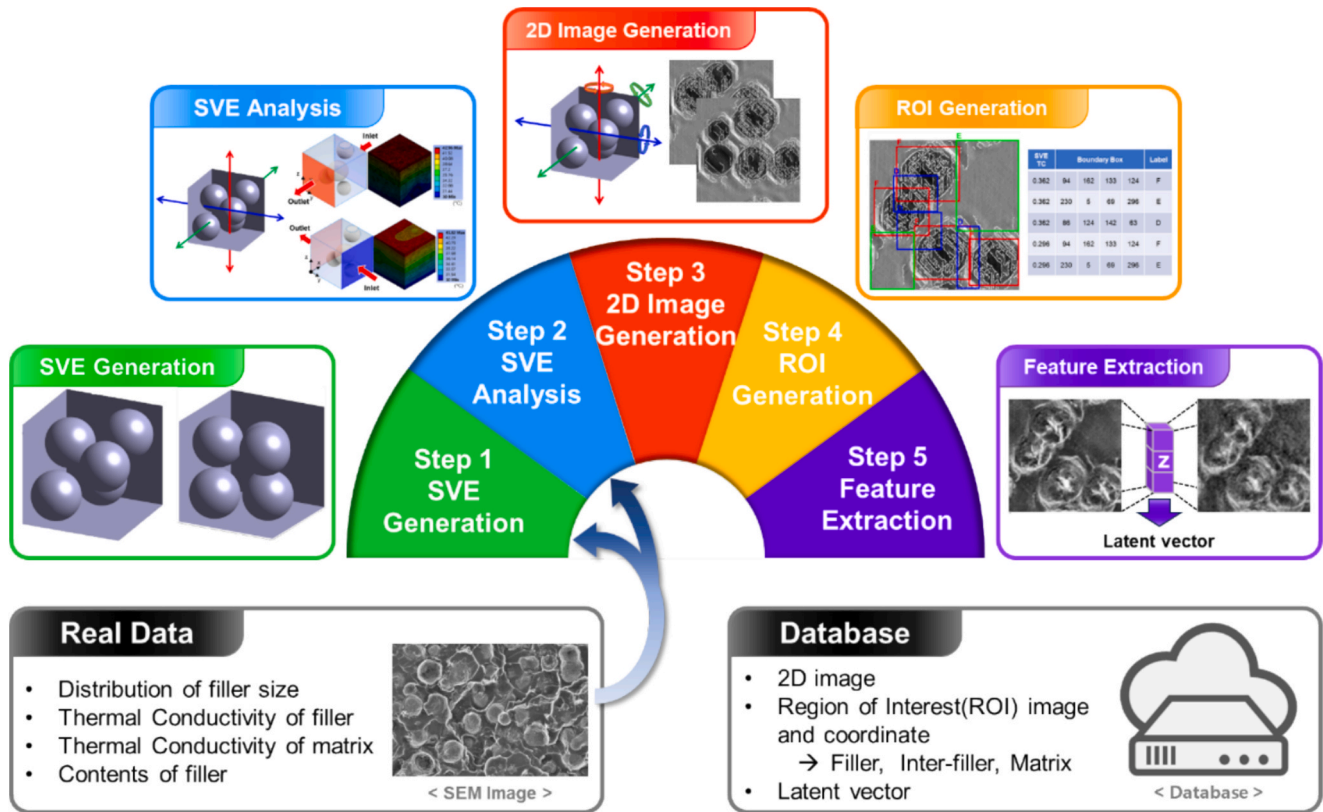


Fig. 1. Simulation-based microstructural database generation process.

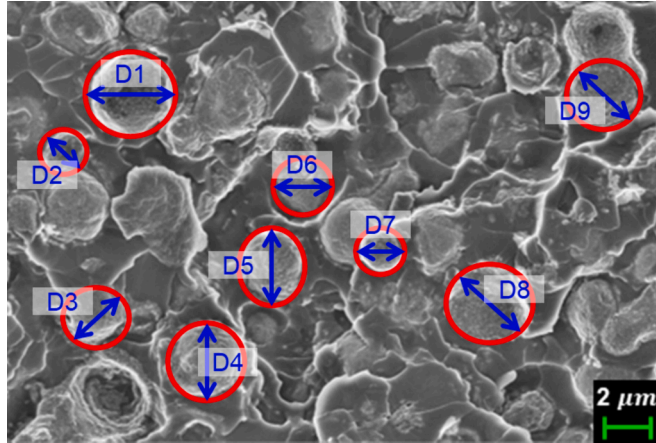


Fig. 2. Measurement of filler size distribution using SEM images. Nine representative filler particles (D1–D9) were identified and measured; blue arrows indicate particle diameters; red circles highlight the boundaries of each filler; and the scale bar represents 2  $\mu\text{m}$ . (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

of the spherical copper powder HACU-025 provided by Chang Sung Corporation (CSC).

Accordingly, the structures shown in Fig. 3 were generated using filler volume fractions ranging from 5 % to 40 %. This range was selected based on the densest practically achievable packing conditions using spherical copper fillers and corresponds approximately to 28 %–84 % in weight fraction, depending on the material densities (e.g., copper and epoxy). This range is consistent with previously reported filler mass fractions used in thermally conductive polymer composites, as summarized in recent review articles [36,37]. To simulate the partial filler

exposure commonly observed in experimental SEM images, we constructed SVEs with particles placed near domain boundaries as shown by the red circles in Fig. 3. These configurations effectively mimic the partial exposure patterns seen in SEM images.

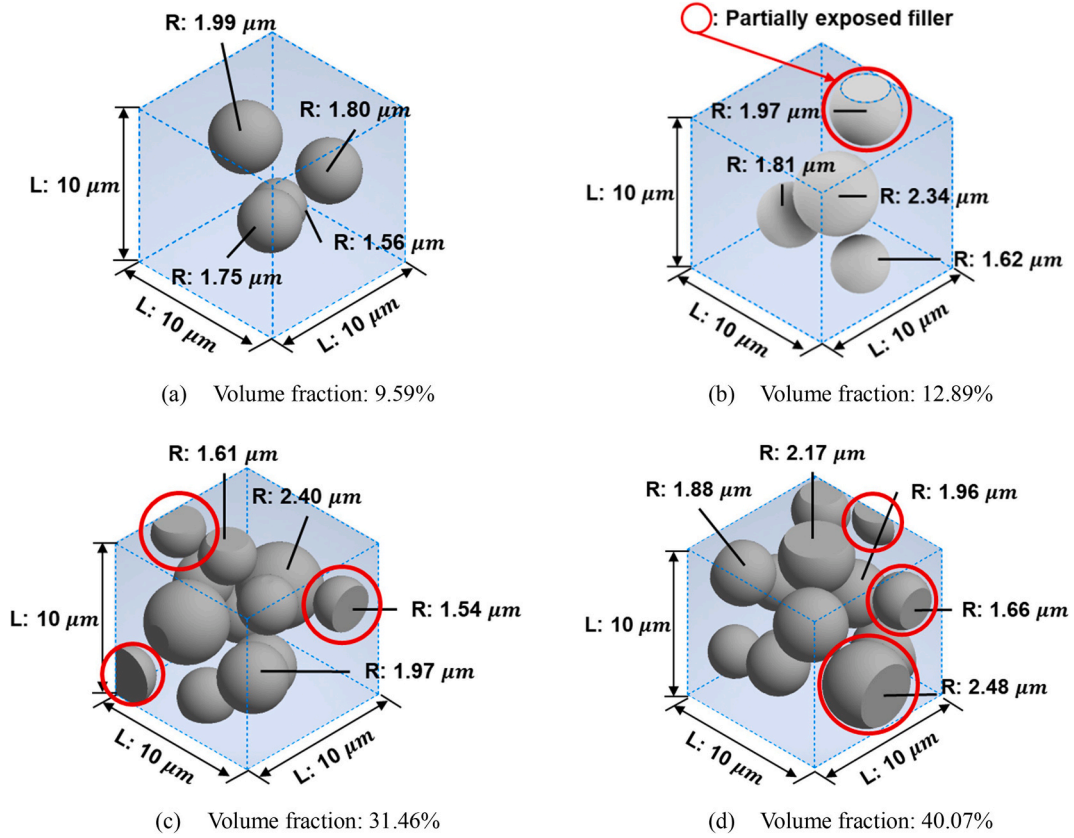
#### 4. Thermal conductivity analysis of SVEs

##### 4.1. Kapitza resistance

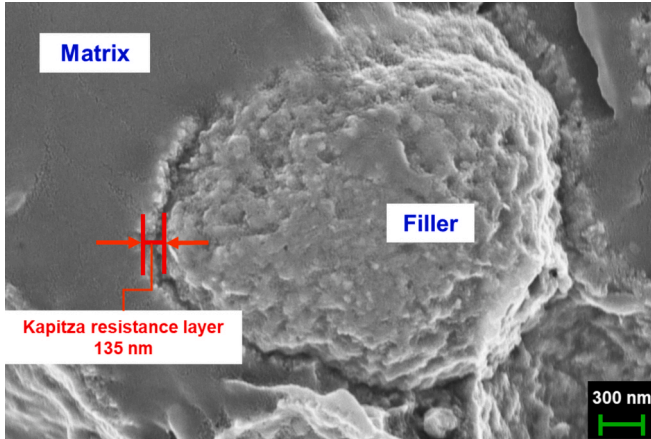
In composite microstructures, the Kapitza resistance is observed at the interfaces between the filler and matrix phases and serves as a major factor influencing the overall heat transfer characteristics. This interfacial resistance became increasingly significant as the filler size decreased owing to the growing relative influence of the interfacial area. In this study, the thickness of the Kapitza resistance layer was quantitatively estimated based on actual SEM images, as shown in Fig. 4. An average thickness of 135 nm was uniformly applied for all fillers. This approach allows interfacial effects to be incorporated into the simulation without explicitly modeling the resistance layer as a separate geometric entity.

Each filler was modeled as a core–shell structure, where the core represented the filler material and the shell simulated the Kapitza resistance layer. Based on this structure, the effective thermal conductivity of each filler was calculated using the Maxwell–Garnett model [19], which is a variant of EMT. Subsequently, the computed effective thermal conductivities were directly assigned to each filler domain within the Ansys model, enabling the simulation to account for interfacial resistance effects in a simplified but physically meaningful manner.

The thermal conductivity of the Kapitza resistance layer was not directly measured in this study but was instead determined by referencing values commonly reported in literature on interfacial thermal resistance in polymer–metal composites [38–40]. Using these literature-derived values, the interfacial thermal-barrier effect was incorporated in a computationally efficient and physically consistent manner, without



**Fig. 3.** Visualization of SVE structures generated with varying filler radii and volume fractions. Models (a) and (b) correspond to volume fractions of 9.59% and 12.89%, respectively, while models (c) and (d) represent denser configurations with 31.46% and 40.07% volume fractions. The red circles indicate partially exposed filler particles. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)



**Fig. 4.** Measurement of the Kapitza resistance layer.

the need to model the interfacial layer as a distinct geometric domain.

#### 4.2. SVE simulation

The thermal conductivity analysis of the generated SVEs was performed using the steady-state thermal module within the commercial finite element software Ansys®. In the simulations, copper (HACU-025), a representative metallic filler, was employed, and YD-128 epoxy resin was used as the matrix material. This material pairing was selected as a representative example to validate the proposed approach; however, the methodology can be readily extended to other spherical filler–matrix

systems. The thermal conductivities of copper and YD-128 epoxy were set to 400 W/m·K and 0.281 W/m·K, respectively.

The simulation assumed steady-state heat conduction. A Dirichlet boundary condition (fixed temperature) was applied to the bottom surface of the SVE model, whereas a Neumann boundary condition (specified heat flux) was imposed on the top surface, with the heat flowing downward. The applied heat flux was fixed at  $Q = 2.5e-7$  W, simulating the thermal behavior under constant heat input, as shown in Fig. 5.

Furthermore, each filler embedded within the SVE was assigned a size-dependent effective thermal conductivity, which was calculated using the Maxwell–Garnett model. These values were individually applied to each filler, allowing the simulation to capture the structural heterogeneity of the system.

Based on the simulation results, the effective thermal conductivity of each SVE was calculated using the temperature difference  $\nabla T$  between the top and bottom surfaces, as follows:

$$K_{sve} = \frac{Q \cdot L}{A \cdot \nabla T} \quad (1)$$

where  $Q$  is the applied heat flux (W),  $L$  is the length in the direction of heat flow,  $A$  is the cross-sectional area through which the heat passes, and  $\nabla T = T_{top} - T_{bottom}$  represents the temperature difference between the two surfaces. The values of  $T_{top}$  and  $T_{bottom}$  were obtained as the average temperatures over the top and bottom surfaces, respectively, to account for the nonuniform temperature distributions across those surfaces.

Thermal simulations were conducted in both the positive (+) and negative (−) directions of the  $x$ ,  $y$ , and  $z$  axes, resulting in six directions for each SVE.

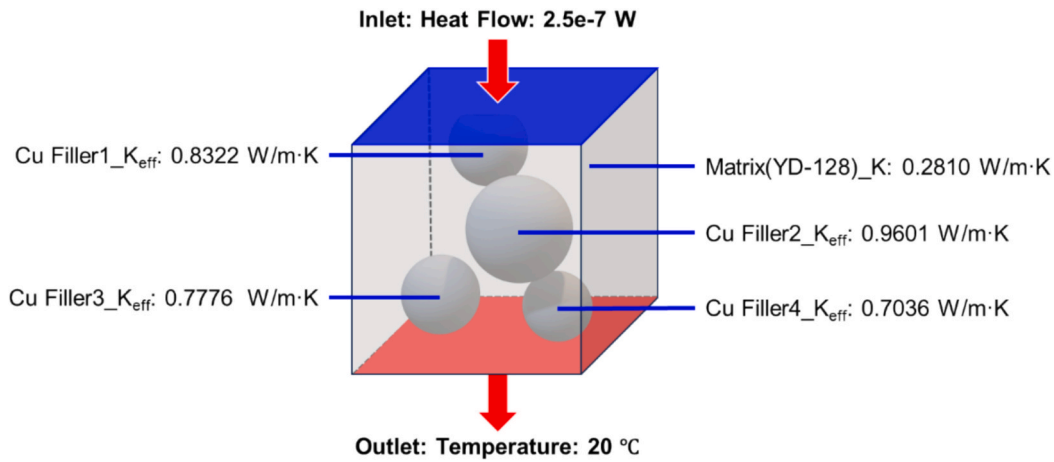


Fig. 5. Boundary conditions and applied heat flux configuration for the steady-state thermal analysis of SVE model.

As shown in Fig. 6, even with the same microstructure, the effective thermal conductivity varied depending on the heat flow direction, indicating anisotropic thermal behavior. This directional variation is not a numerical artifact but a structurally induced phenomenon, arising from subtle differences in filler connectivity and alignment along each axis. Although geometrically symmetric SVEs and boundary conditions were applied, the stochastic nature of filler distribution induces local anisotropy, resulting in direction-dependent thermal conductivity. This

effect was consistently observed across multiple SVEs and rotational configurations. This simulated anisotropy has also been reported in other experimental studies [41,42], which show that aligning thermally conductive fillers along the heat flow direction significantly improves the thermal conductivity of polymer composites. (Fig. 7).

The results summarized in Table 1 clearly show that, even under an identical microstructural configuration (identical SVE structure), the thermal behavior exhibits directional anisotropy depending on the heat

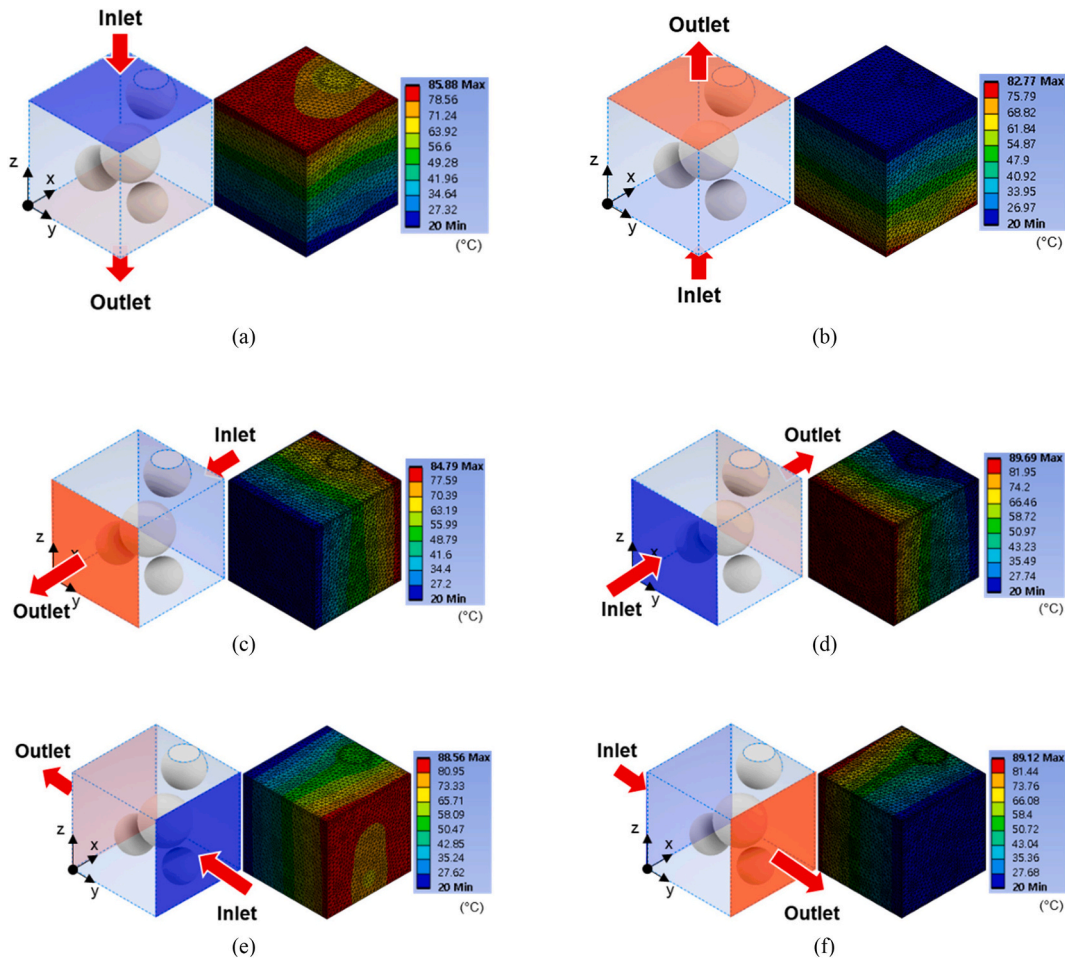
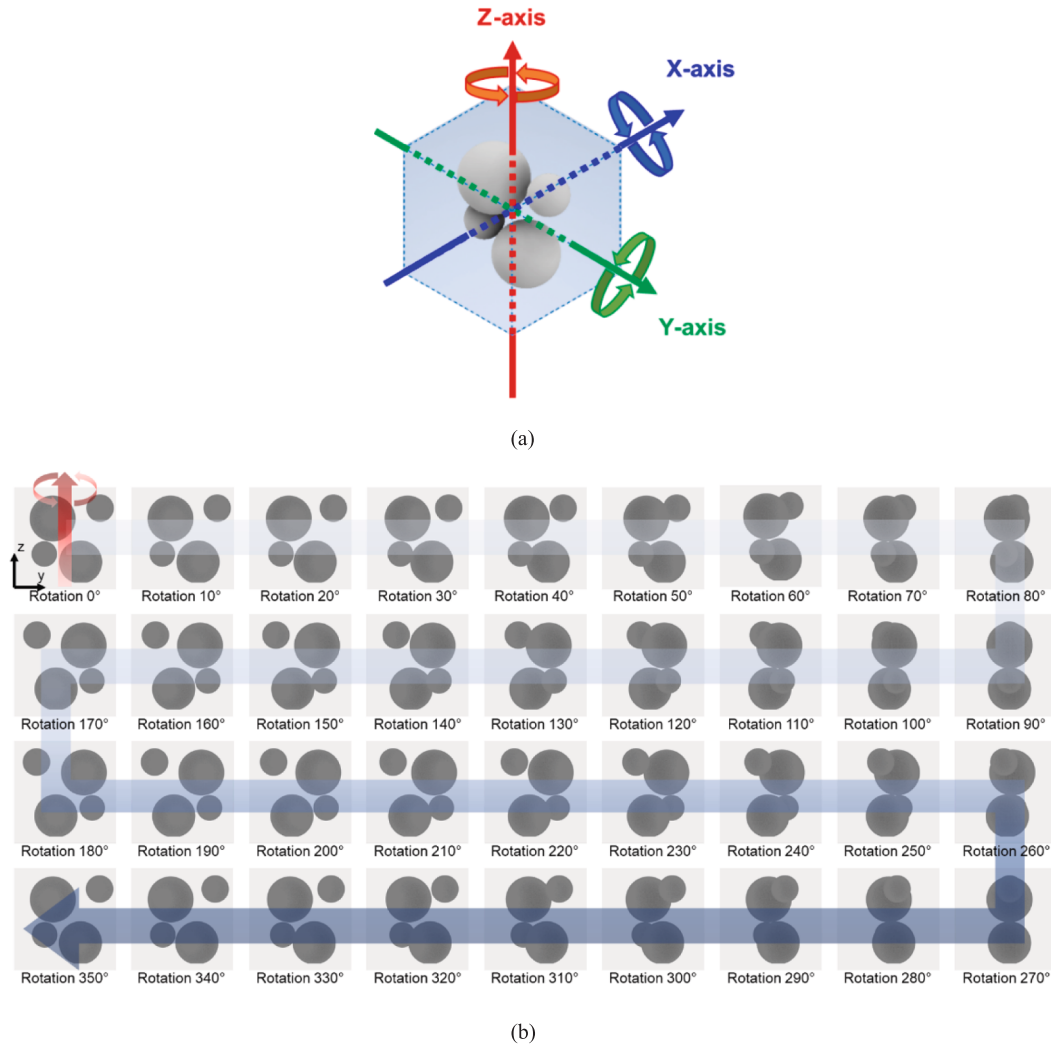


Fig. 6. Comparison of temperature distributions under different heat flow directions for the same SVE: (a)  $+z \rightarrow -z$ ; (b)  $-z \rightarrow +z$ ; (c)  $+x \rightarrow -x$ ; (d)  $-x \rightarrow +x$ ; (e)  $+y \rightarrow -y$ , (f)  $-y \rightarrow +y$ .



**Fig. 7.** 3D axis-specific rotation and orientation-augmented 2D image generation: (a) Schematic of the 3D coordinate system and axis-specific rotation directions applied to SVE structures; rotations were performed independently around the X-axis (blue), Y-axis (green), and Z-axis (red) to generate diverse orientations. (b) Example of orientation augmentation by successive rotations around the Z-axis at 10° increments, demonstrating variation in 2D projections captured from rotated SVE structures. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

**Table 1**  
Temperature and thermal conductivity results.

| Heat Flow Direction | Max Temperature (°C) | Min Temperature (°C) | Average Temperature (°C) | Thermal Conductivity (W/m·K) |
|---------------------|----------------------|----------------------|--------------------------|------------------------------|
| +z → -z             | 85.88                | 64.48                | 78.06                    | 0.431                        |
| -z → +z             | 82.77                | 61.25                | 76.52                    | 0.442                        |
| +x → -x             | 84.79                | 79.03                | 81.68                    | 0.405                        |
| -x → +x             | 89.69                | 73.24                | 85.48                    | 0.382                        |
| +y → -y             | 88.56                | 72.37                | 83.00                    | 0.397                        |
| -y → +y             | 89.12                | 71.45                | 83.30                    | 0.395                        |

flow orientation. Specifically, noticeable differences can be observed in the maximum, minimum, and average surface temperatures and in the calculated effective thermal conductivity values across different heat conduction directions. These findings indicate that the formation and continuity of the internal heat transfer pathways are strongly influenced by the orientation of the microstructure relative to the thermal flux direction, which gives rise to direction-dependent (anisotropic) thermal transport characteristics in the composite.

## 5. 2D image generation

### 5.1. Rotational data augmentation

The direction-dependent variability highlights the anisotropic nature of thermal transport in the material. To incorporate this anisotropic behavior into model training, each 3D SVE was visualized from six different heat conduction directions, corresponding to  $\pm x$ ,  $\pm y$ , and  $\pm z$ . For each direction, a 2D image was generated to reflect the microstructural configuration aligned with that specific thermal conduction path. The effective thermal conductivity obtained from the simulation in this direction was assigned as the ground-truth label for the corresponding 2D image.

In addition to directional variations, rotational transformations were systematically applied to each SVE around the principal axes. Unlike changing the heat flow direction, this operation rotates the SVE itself and therefore does not alter its thermal conductivity. However, by visualizing the same structure from different orientations, it generates 2D images with distinct visual appearances. Although the underlying filler arrangement remains unchanged, the perceived structure varies depending on the viewing angle.

In some cases, fillers appear partially occluded by other overlapping

particles, making only fragments visible. This visual occlusion mimics how rough and uneven surfaces in SEM images obscure the overall shape of fillers. By learning to associate such partial visual cues with complete geometries, the model becomes more robust to partial particle exposure in 2D representations of 3D structures.

The dataset captures a wide spectrum of spatial and geometric variations by combining directionally varied image views and rotational augmentations. This setup allows the model to learn structure–property relationships more effectively, particularly in terms of the influence of microstructural features such as the filler distribution, connectivity, and orientation on the overall thermal behavior.

### 5.2. Image transformation

The generated morphological images were structurally accurate but lacked the visual complexity typically observed in actual experimental data. Specifically, these images exhibit idealized contrast, smooth textures, and sharply defined boundaries—features that are rarely present under actual imaging conditions. To reduce the visual gap between the simulated and experimental data and enhance the generalizability of the model, the simulation images were further transformed to resemble the SEM images of actual composite materials.

To achieve this visual transformation, a style transfer method based on CycleGAN [43] was employed. The objective was to embed features that are frequently observed in SEM images, such as irregular surface textures, diffuse and stochastic noise, and high-contrast but imperfect boundaries between the filler and matrix regions. By incorporating these realistic visual artifacts, the dataset was enriched to reflect the uncertainties inherent in experimental observations, allowing the model to better adapt to imperfect and noisy inputs.

However, when CycleGAN was applied directly to the raw simulation images without any preprocessing, the generated SEM-like images, such as the example derived from the original SVE 2D image shown in the lower-left corner of Fig. 8, frequently exhibited structural distortions and unnatural textures. These artifacts limit the utility of the images as

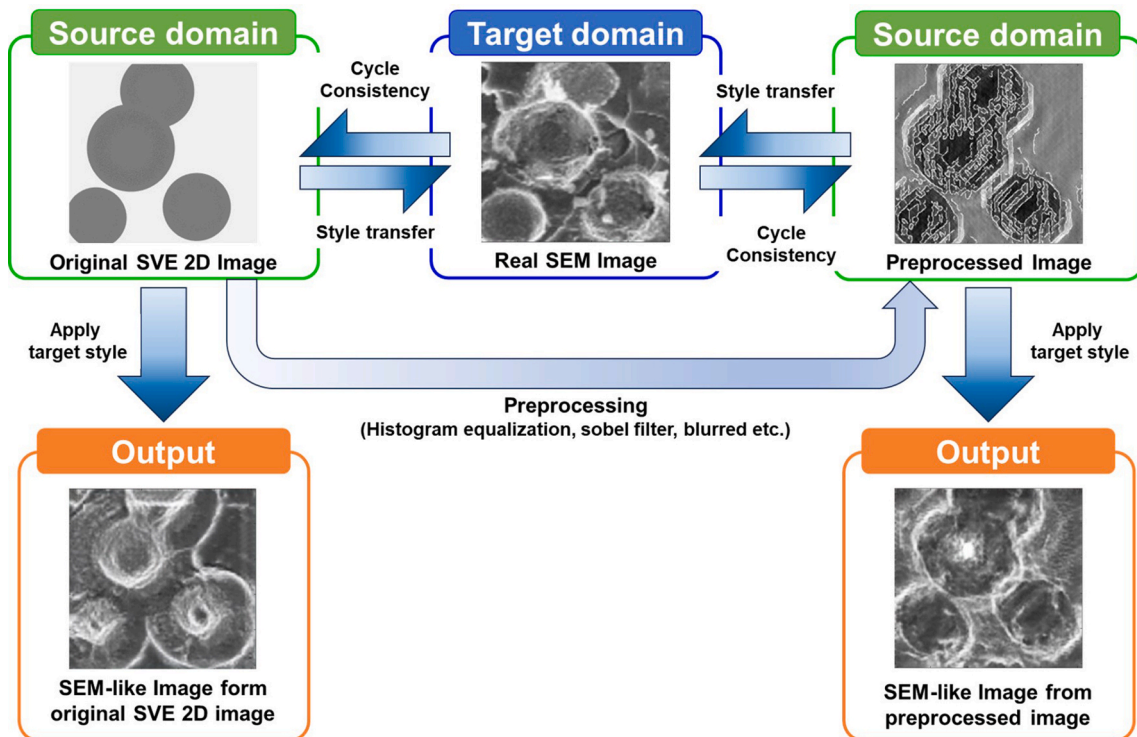
realistic training data because they fail to replicate the key stylistic elements of SEM images, including accurate surface texture, filler morphology, and noise patterns.

To address these limitations, a dedicated preprocessing pipeline was introduced prior to CycleGAN training. The purpose of this pipeline was to preserve the structural integrity of the simulation images while gradually incorporating SEM-like visual characteristics to improve style transfer stability and effectiveness. First, histogram equalization was applied to mitigate the overly uniform brightness in the simulation outputs and normalize global contrast. This step introduces heterogeneous intensity patterns similar to those observed in actual SEM images. Next, edge enhancement was performed using a Sobel filter to sharpen the boundaries between the filler and matrix regions, where CycleGAN tends to blur during transformation. Additionally, Gaussian noise was added to simulate the random pixel intensity fluctuations that are typically caused by electron scattering and Gaussian blurring was applied to reproduce subtle defocus effects. Together, these preprocessing steps can generate input images that reflect the visual characteristics of SEM images more accurately, facilitating more effective domain adaptation using CycleGAN.

The resulting SEM-like images, shown in the lower-right corner of Fig. 8, exhibit significantly improved visual realism and structural fidelity. These enhanced images were used as training inputs for the CNN-based thermal conductivity prediction model, contributing to the more accurate learning of complex structure–property relationships in composite materials.

To verify that the CycleGAN outputs are statistically consistent with real SEM micrographs, the Fréchet Inception Distance (FID) was computed between the two image sets, each comprising 187 images. FID embeds every image in the 2,048-dimensional pool-3 feature space of Inception-v3 and measures the distance between the corresponding multivariate Gaussian distributions:

$$FID = \|\mu_r - \mu_g\|^2 + \text{Tr} \left( \Sigma_r + \Sigma_g - 2(\Sigma_r \Sigma_g)^{\frac{1}{2}} \right) \quad (2)$$



**Fig. 8.** Effect of source image preprocessing on CycleGAN-based style transfer. SEM-like outputs generated from preprocessed inputs exhibit improved texture, contrast, and structural consistency compared with outputs from raw simulation images.

where  $\mu_r$  and  $\Sigma_r$  represent the mean vector and covariance matrix of the real SEM image set, while  $\mu_g$  and  $\Sigma_g$  represent those of the generated image set, and  $T_r(\bullet)$  denotes the matrix trace, which aggregates total variance. Using the fixed SEM reference set, the CycleGAN trained on raw simulation images produced an FID of 7.13, whereas the proposed preprocessing pipeline achieved an FID of 1.34, corresponding to an approximately 81 % reduction in distributional divergence.

## 6. ROI generation

An ROI is a localized microstructural area within an image that significantly influences the thermal conductivity of a composite material. In the proposed framework, ROI information is incorporated as an auxiliary input to allow the model to learn the quantitative relationship between microstructural characteristics and thermal behavior accurately. The ROIs are categorized into three classes: filler regions (F), inter-filler gaps (D), and matrix regions without fillers (E).

To ensure that subtle spatial correlations, such as filler–filler spacing gradients, are not overlooked when defining ROIs, the selection strategy was carefully designed to include not only filler-containing regions but also inter-filler transition zones and matrix-only areas. This design choice reflects the understanding that not only the presence of fillers, but also their spatial arrangement and surrounding matrix patterns, critically affect thermal conduction. Such broader coverage enables the model to capture more continuous and physically meaningful structural contexts across the microstructure.

Each ROI is automatically detected using a bounding box-based method powered by Faster R-CNN, which is a deep learning-based object detection algorithm. This classification is supported not only by physical intuition but also by empirical results from thermal simulations of various SVE structures. The simulations confirmed that, in addition to the filler location and density, the spatial arrangement of the inter-filler gaps and distribution patterns of the matrix regions also play an important role in determining the overall thermal conductivity of the material.

To effectively integrate such localized structural diversity into the model, each ROI was encoded with its corresponding class label ('F', 'D', or 'E') along with its spatial coordinates in the form of (x, y, width, height). This information was used as an auxiliary input independent of the full image, allowing the model to learn global structural patterns and localized morphological features simultaneously. Fig. 9 illustrates an example of the ROI configuration employed in this study. The figure shows that the bounding boxes are overlaid on an SEM-like image generated by CycleGAN, with each box automatically annotated by

Faster R-CNN and labeled as one of the three ROI classes. In addition to the class label, the bounding box contains precise coordinate information, allowing for a quantitative definition of key microstructural elements.

Instead of treating these bounding box annotations as metadata, the proposed approach actively utilizes them by cropping each ROI into image patches. Subsequently, these patches are used as separate inputs for the multi-input CNN. The ROI images for each class are provided via different input channels, allowing the model to independently learn the structural characteristics of each microstructural component. Moreover, the bounding box coordinates and class labels are provided as auxiliary inputs, allowing the model to integrate both visual features and quantifiable spatial data linked to each ROI. To complement the spatial representation of the entire image, a latent vector is extracted using an autoencoder to capture high-level structural representations. The implementation and role of the latent vector are discussed in the following section.

## 7. Feature extraction

CNNs are inherently well-suited for capturing localized spatial features, such as the distribution, shape, and boundaries of fillers and matrix regions within composite images. However, CNNs often face challenges in capturing broader contextual relationships or global structural patterns that extend beyond local receptive fields. This limitation can be particularly critical in microstructural analysis, where composite thermal behavior is governed not only by the local geometry but also by higher-order spatial arrangements and interactions across the entire image domain.

To complement the CNN's ability to capture local features, we incorporated an autoencoder to extract global structural characteristics from the entire microstructure image. The resulting 512-dimensional latent vector serves as a compact and nonlinear embedding that encodes high-level spatial features relevant to thermal transport. While the individual latent dimensions are not physically interpretable, the overall representation captures essential global patterns that critically influence the formation of continuous thermal pathways. These latent vectors are provided as auxiliary inputs to the model, enhancing its capacity to learn complex structure–property relationships.

During the implementation process, the latent dimensions of the autoencoder were predefined and optimized. The autoencoder was trained using the entire image dataset. Each image  $X$  was encoded into a latent vector  $Z$  and then decoded to reconstruct an approximation  $\hat{X}$  of the original image. The training objective was to minimize the reconstruction error, which was quantified using a combination of loss

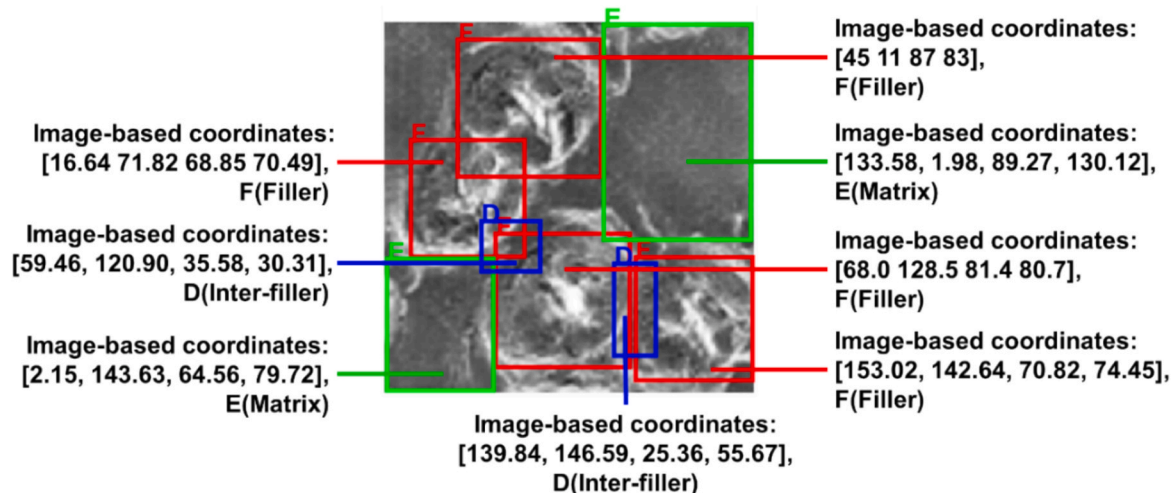


Fig. 9. Visualization of bounding boxes for D, E, and F classes on generated SEM-like image.

functions, such as the mean squared error (MSE) and structural similarity index measure (SSIM), which assesses pixel-level accuracy in addition to perceptual and structural fidelity.

Various latent-space sizes were tested to select the optimal latent dimension, and the quality of the reconstructed images was evaluated. As expected, increasing the dimensionality generally led to improved reconstruction accuracy. Ultimately, a latent dimension of 512 was selected because it provides the best balance between representational richness and dimensional efficiency. Fig. 10 shows a qualitative comparison of the reconstruction performance across different latent dimensions, highlighting the improvements in structural preservation and visual fidelity as the latent space increases.

The final latent vectors obtained via this process serve as compact representations of the essential features of each image and are used as auxiliary inputs in the proposed model to enhance the learning of complex structure–property relationships.

## 8. Multi-input CNN

In this study, a multi-input CNN-based regression model was developed to predict the thermal conductivity of composite materials using 2D images. The model was designed to learn multiple features that influence thermal conductivity, including the global structural characteristics of the entire image, local features from ROIs, and the spatial information of each ROI. This allows the model to more accurately capture the influence of microstructural variations, such as filler distribution, size, and spacing, on the thermal behavior of composites.

The model uses five types of input data:

1. 2D base image generated from rotated SVE structures;
2. ROI images for three distinct classes, with each class provided as a separate input channel;
3. ROI coordinates for each class;
4. ROI class labels corresponding to each ROI image; and
5. latent vector extracted from the autoencoder to represent the low-dimensional embedding of global image features.

Although five types of input data exist, some types, namely ROI images, coordinates, and class labels, are handled separately per class. Consequently, the model contains multiple input layers to accommodate each class-specific input branch. During model training, the thermal conductivity corresponding to each input set obtained from the thermal analysis described in Section 4 was used as the regression target and served as the ground truth. Each input type was processed using a dedicated branch of the network.

The full and ROI images were passed through the CNN layers to extract spatial features, whereas the ROI coordinates and class labels were processed using fully connected layers. Subsequently, the extracted features were merged using a concatenation layer and the combined feature vector was passed through additional fully connected layers to predict the final thermal conductivity. Fig. 11 illustrates the architecture of the proposed multi-input CNN. The network independently processed each input type, extracted meaningful features, and fused them for

regression. This design allows the model to learn both global and local microstructural characteristics, resulting in more accurate and robust thermal conductivity prediction across a range of composite configurations.

To further enhance the stability and generalization of the predictions, Huber robust regression was applied to the outputs of the trained multi-input CNN model as a post-processing step. This improved the reliability and accuracy of the final thermal conductivity predictions by reducing the influence of potential outliers on the training data [44].

In this study, 1,728 datasets were generated to predict the thermal conductivities of the composite materials. Each dataset comprised a 2D SVE image and its corresponding thermal conductivity value. The entire dataset was split into training (80 %), validation (10 %), and testing (10 %) sets. The SVEs were constructed with filler volume fractions ranging from 5 % to 40 %, allowing controlled microstructural density variation. The thermal conductivity values ranged from 0.362 W/m·K to 0.560 W/m·K, covering 29 distinct values in total. The mean thermal conductivity was 0.441 W/m·K with a standard deviation of 0.052 W/m·K. Although the overall distribution spans a relatively narrow range of thermal conductivity values, it encompasses a finely resolved set of variations, thereby allowing the model to learn and distinguish subtle variations in the influence of microstructure on thermal transport. Each generated 2D SVE image contained ROIs, which are considered key structural elements that influence the thermal conductivity of the composite. On average, each image included 11.58 ROIs, with the class-wise average counts being 5.28 for class F, 4.46 for class D, and 1.85 for class E.

## 9. Validation results

To validate the performance of the proposed multi-input architecture and conduct a quantitative analysis of the contribution of each input component to the model's prediction of the model, six different experiments were designed based on varying input configurations. The experiments followed a structured progression, beginning with a baseline model using only the full image as input and sequentially incorporating ROI images, ROI coordinates, class information, and a latent vector extracted from the autoencoder. The configurations are defined as follows:

Configuration #1: Full image only.

Configuration #2: Full image + ROI images.

Configuration #3: Full image + latent vector.

Configuration #4: Full image + ROI images/coordinates/class.

Configuration #5: Full image + ROI images/coordinates/class + latent vector (without robust regression).

Configuration #6: Full image + ROI images/coordinates/class + latent vector (with robust regression).

To perform a quantitative assessment of the effectiveness of the proposed multi-input CNN architecture, the regression performance was compared across six input combinations. The experiment used 10 % of the dataset reserved for testing and was designed to evaluate the incremental impact of each input feature on the prediction accuracy by sequentially expanding the input configuration from a basic full image input to the inclusion of ROI images, ROI coordinates, class labels, and a

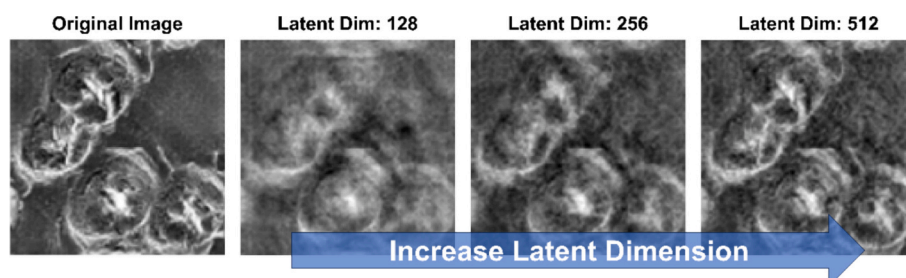
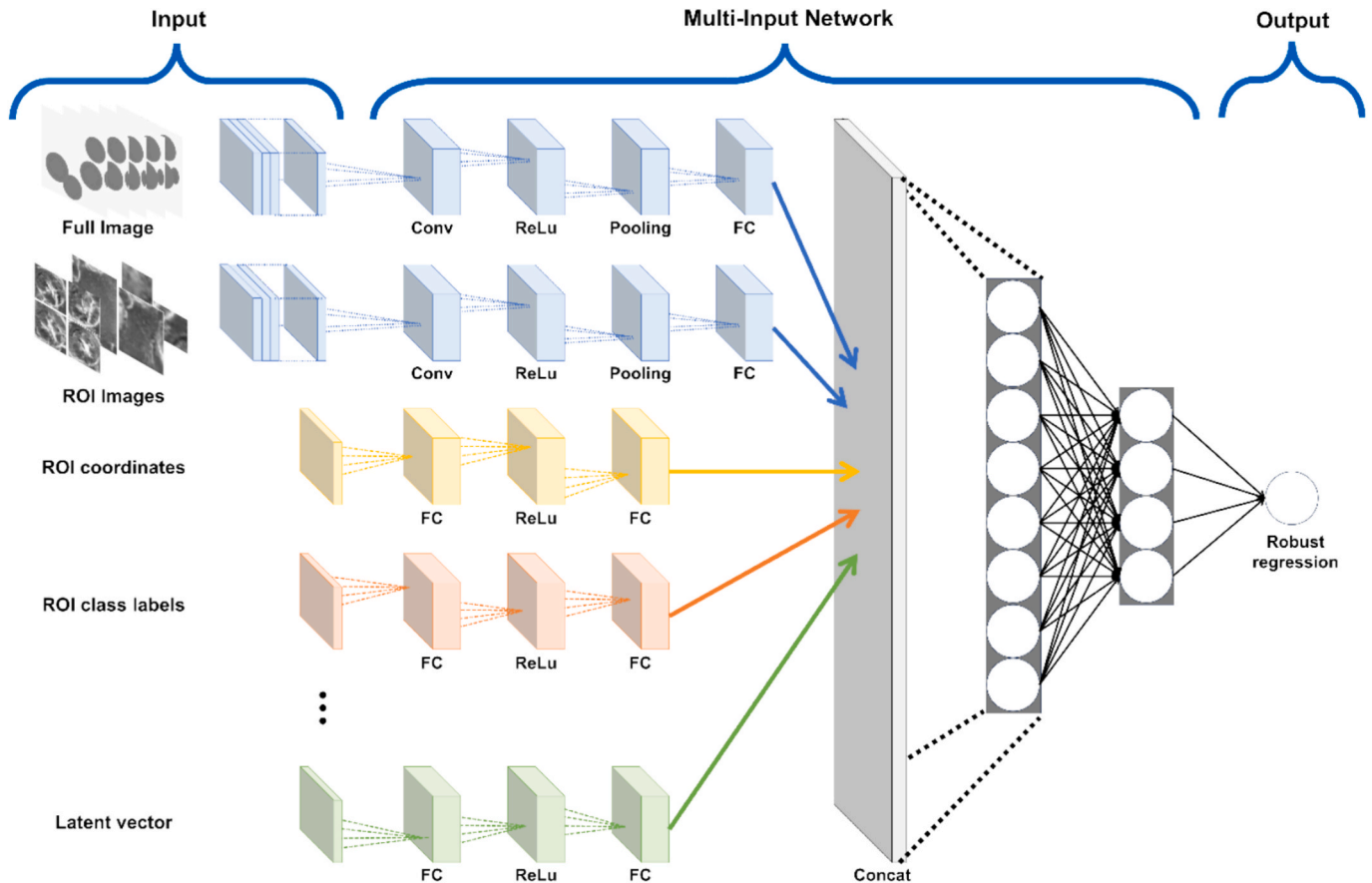


Fig. 10. Comparison of the original image and decoded results according to latent dimension.



**Fig. 11.** Architecture of the proposed multi-input CNN. For each ROI, the corresponding cropped image, coordinate, and class label are processed independently. The model supports multiple ROIs per input image.

latent vector extracted by an autoencoder. To ensure robust evaluation, each training session involved a randomized data split. Since the specific samples included in the training and validation sets vary with each split, the model may learn slightly different feature patterns, leading to variations in performance. Therefore, all reported metrics represent the average results over multiple independent runs.

As presented in Table 2, Configuration #1 (full image only) resulted in the worst performance, with  $\text{RMSE} = 0.7809$  and  $R^2 = -8.6277$ , indicating that the model failed to capture a meaningful correlation between the predicted and actual thermal conductivity values. This suggests that the full image data alone do not sufficiently represent the key structural features that influence thermal conductivity.

Configuration #2 (full image + ROI images) achieved a slight improvement, with  $\text{RMSE} = 0.2052$  and  $R^2 = 0.3603$ . The inclusion of ROI images contributed additional local structural information related to heat transfer-sensitive regions, partially enhancing the prediction capability.

**Table 2**

Comparison of prediction performance of different input configurations in the proposed multi-input CNN model.

| Config. # | Input Configuration Description                                                       | RMSE   | $R^2$   |
|-----------|---------------------------------------------------------------------------------------|--------|---------|
| 1         | Full Image only                                                                       | 0.7809 | -8.6277 |
| 2         | Full Image + ROI Images                                                               | 0.2052 | 0.3603  |
| 3         | Full Image + Latent Vector                                                            | 0.1148 | 0.7974  |
| 4         | Full Image + ROI Images/Coordinates/Class                                             | 0.1532 | 0.6200  |
| 5         | Full Image + ROI Images/Coordinates/Class + Latent Vector (without robust regression) | 0.0848 | 0.8923  |
| 6         | Full Image + ROI Images/Coordinates/Class + Latent Vector (with robust regression)    | 0.0664 | 0.9315  |

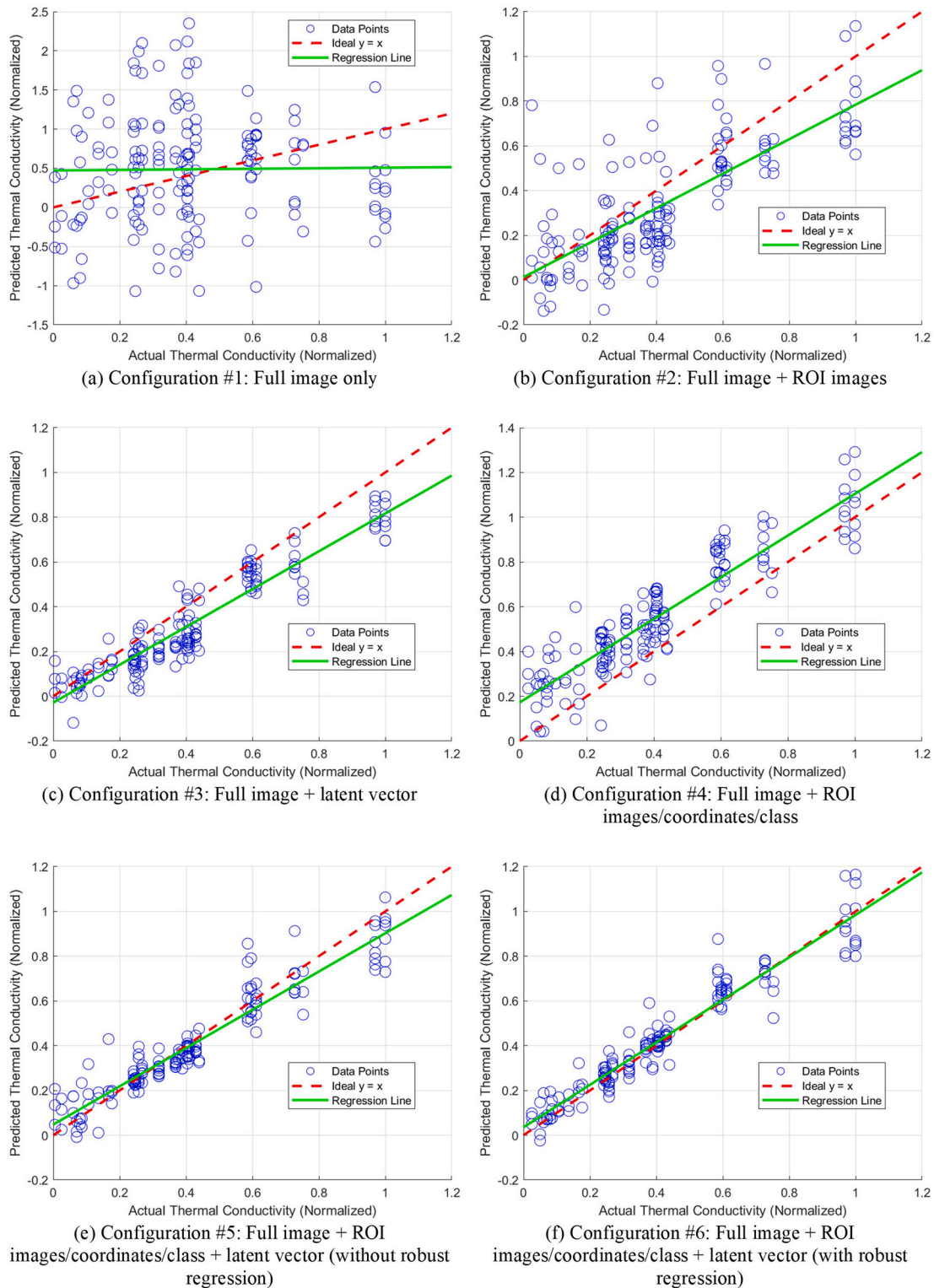
In Configuration #3 (full image + latent vector), substantial performance improvement was observed ( $\text{RMSE} = 0.1148$  and  $R^2 = 0.7974$ ). This highlights the importance of global structural patterns that are effectively captured in the latent representation extracted by the autoencoder. Although this configuration did not yield the best overall performance, it significantly outperformed earlier configurations without relying on ROI information, demonstrating that the latent vector alone provides a strong and informative global representation of the microstructure.

In Configuration #4 (full image + ROI images/coordinates/class): The ROI images were supplemented with their spatial positions and class labels. This led to moderate performance improvement ( $\text{RMSE} = 0.1532$  and  $R^2 = 0.6200$ ), supporting the hypothesis that adding contextual information for local features improves interpretability, even though it still falls short of the performance achieved by the latent vector-based model.

Configuration #5 (full image + ROI images/coordinates/class + latent vector without robust regression) combined both global (latent vector) and refined local features (ROI, coordinates, and class) to achieve strong performance ( $\text{RMSE} = 0.0848$  and  $R^2 = 0.8923$ ). This demonstrates the benefit of integrating both levels of structural representation to enhance prediction accuracy.

Configuration #6 (with robust regression) achieved the best performance across all configurations ( $\text{RMSE} = 0.0664$  and  $R^2 = 0.9315$ ). The robust regression step mitigated the influence of outliers in the training data and provided more stable and reliable predictions. As illustrated in Fig. 12, the values predicted from this configuration closely align with the ground truth.

These results clearly demonstrate that the combination of local information (ROI images, coordinates, and classes) and global features



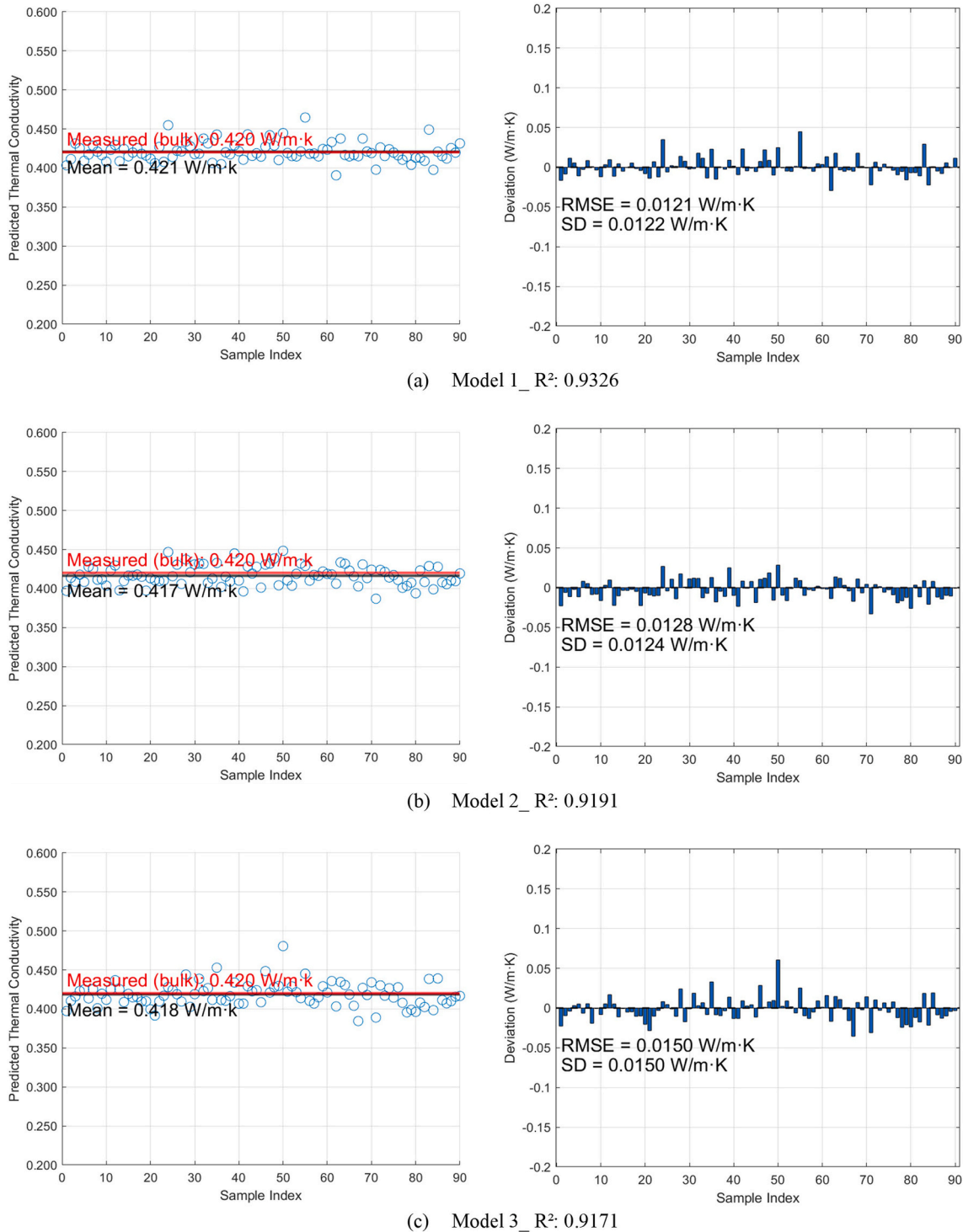
**Fig. 12.** Prediction results for each input configuration of the proposed multi-input CNN model. The green line represents the regression result and the red dashed line represents the ideal  $y = x$ . (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

(latent vectors) is critical to enhancing model performance in predicting the thermal conductivity of composites. In particular, relying solely on the full image input is insufficient, whereas incorporating ROI-based structural cues enables the model to capture heat-sensitive regions more precisely. Furthermore, the latent vector effectively summarizes the global characteristics of the microstructure, thereby significantly improving the model's generalization capability.

To validate the performance of the trained model, an actual SEM image obtained from a bulk-scale composite specimen was employed. The specimen used for validation was fabricated using the same constituents, with the filler content set to approximately 12 vol%. The SEM image was cropped to match the input size used during training, and the same preprocessing and feature extraction pipeline was applied. The thermal conductivity of the specimen was measured five times using an

LFA (Laser Flash Apparatus)-457 instrument, and the average of these measurements was 0.420 W/m·K. The LFA-457 is known to have a reported measurement uncertainty of approximately  $\pm 5.6\%$ . Fig. 13 compares the prediction results on an actual SEM image using multiple models trained on different randomized data splits. As previously

discussed, variations in the sampled training data can lead each model to learn slightly different features, resulting in minor prediction differences. The predicted values ranged from 0.417 to 0.421 W/m·K, with an average of 0.419 W/m·K. The RMSE and SD were calculated as 0.0133 and 0.0132, respectively. This result highlights the practical potential of



**Fig. 13.** Predicted thermal conductivity values obtained by applying the trained CNN model to SEM images of an actual composite. The red line indicates the experimentally measured bulk-scale thermal conductivity (0.420 W/m·K) of the fabricated specimen, while the blue dots represent predictions based on microstructural features captured in the SEM image. Results are shown for three independently trained models using different randomized training data splits: (a) Model 1 achieved an  $R^2$  of 0.9326, with a mean prediction of 0.421 W/m·K, RMSE of 0.0121 W/m·K, and SD of 0.0122 W/m·K (b) Model 2 achieved an  $R^2$  of 0.9191, with a mean prediction of 0.417 W/m·K, RMSE of 0.0128 W/m·K, and SD of 0.0124 W/m·K (c) Model 3 achieved an  $R^2$  of 0.9171, with a mean prediction of 0.418 W/m·K, RMSE of 0.0150 W/m·K, and SD of 0.0150 W/m·K. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

the proposed framework, demonstrating that meaningful property predictions can be achieved from real micrographs—even when only limited microstructural regions are available. Therefore, the proposed multi-input CNN framework constitutes a robust and effective architecture for learning complex structure–property relationships in composite materials.

## 10. Conclusion

In this study, a thermal-conductivity prediction framework for polymer composites was developed based on 2D SVE images and a multi-input CNN. A rotation-based data augmentation strategy was first employed to generate diverse microstructures from a limited number of SVEs, significantly reducing the computational burden of repeated simulations. The proposed framework integrates local features from heat-sensitive ROIs and global structural representations extracted as latent vectors using an autoencoder. Notably, the latent vector alone achieved solid performance ( $R^2 = 0.7974$ , RMSE = 0.1148), and combining it with ROI-based inputs further improved prediction accuracy ( $R^2 = 0.8923$ , RMSE = 0.0848). Additionally, applying robust regression as a post-processing step mitigated the influence of outliers, resulting in the best performance ( $R^2 = 0.9315$ , RMSE = 0.0664).

To improve real-world applicability, a CycleGAN-based domain adaptation module was introduced to convert idealized simulation images into SEM-like representations, thereby allowing the model to account for noise and irregularities inherent in experimental data. The effectiveness of this transformation was quantitatively validated using the FID, confirming the high similarity between the generated and real SEM images. Furthermore, the trained model was directly applied to an actual SEM image obtained from a bulk-scale composite specimen, and the predicted thermal conductivity—computed as the average over the entire cropped image—deviated by only  $\sim 1\%$  from the experimentally measured value. This result demonstrates that the model is capable of producing reliable predictions even under limited and noisy observational conditions. In addition, the proposed framework effectively captures the influence of critical microstructural factors such as filler distribution, connectivity, and spacing on effective thermal conductivity.

Future research will focus on extending the framework to accommodate anisotropic filler geometries (e.g., platelets, fibers), multiphase composite systems, and 3D microstructures. Moreover, the incorporation of internal voids based on 3D imaging techniques such as X-ray CT is planned to further improve the model's physical fidelity and predictive reliability. We also plan to quantify the noise and artifacts and incorporate them into the modeling process to further enhance the applicability and generalizability of the framework to diverse experimental datasets.

## CRedit authorship contribution statement

**Mingeon Kim:** Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Conceptualization. **Geonhwi Lee:** Software, Investigation, Conceptualization. **Seung-Kyum Choi:** Software, Methodology, Conceptualization. **Hae-Jin Choi:** Writing – review & editing, Writing – original draft, Supervision, Resources, Methodology, Funding acquisition, Conceptualization.

## Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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## Data availability

Data will be made available on request.

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