Endterm Report for SURGE-2023

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Synthetic Microstructure Data Generation for Composite Architecture Prediction

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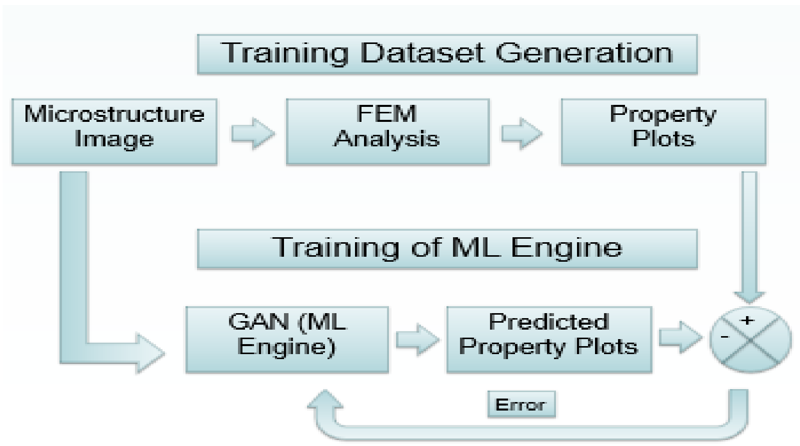
Abstract:

This project focuses on the generation and analysis of synthetic microstructures for predicting property plots of composite materials using machine learning (ML) algorithms. In recent years, data-driven methods have gained prominence in predicting material properties. In this project, the we employed the FEniCS framework, which is a popular computational toolkit for solving partial differential equations, to perform finite element method (FEM) simulations. These simulations were used to generate property plots for composite materials, which served as labeled data for training a Generative Adversarial Network (GAN) model. The GAN model was specifically developed to predict stress intensity and displacement plots for unseen microstructures. GANs are a class of deep learning models that consist of two components: a generator network and a discriminator network. The generator network generates synthetic data samples, in this case, microstructures, while the discriminator network evaluates the authenticity of the generated samples. Through an adversarial training process, the generator learns to produce synthetic microstructures that closely resemble the real ones used in the FEM simulations. The results of this project demonstrated the potential of the GAN model to accurately predict stress intensity and displacement patterns based on synthetic microstructures. This finding is significant for materials engineering as it offers an efficient alternative to physical experiments for generating and analyzing microstructures. By combining the computational capabilities of FEniCS and the generative power of GANs, researchers and engineers can gain new insights into the behavior of composite materials and design them with tailored mechanical properties. Overall, this project showcases the promising intersection of computational simulations, ML algorithms, and materials engineering. It highlights the ability of GAN models to learn and generate complex microstructures, enabling accurate predictions of material properties. The integration of FEniCS and GANs opens up exciting avenues for researchers to explore and understand composite materials at a deeper level, facilitating the development of advanced materials with enhanced mechanical properties and performance.

Introduction:

In the field of materials research and development, understanding the relationship between microstructures and material properties is of paramount importance. The ability to accurately predict material properties under different conditions is crucial for designing new materials with specific desired properties or optimizing existing ones. However, conducting physical experiments to obtain such data can be time-consuming, costly, and sometimes impractical. To overcome these challenges, synthetic microstructure generation has emerged as a valuable tool in materials engineering. By simulating the microstructure of a material, researchers can obtain information about its properties under various conditions without the need for extensive experimental setups. Synthetic microstructures also provide a means to generate large datasets, which are essential for training machine learning models. This research project aims to accelerate materials engineering by combining image processing, computational modeling, and machine learning techniques. The integration of these diverse disciplines enables researchers to simulate and analyze the microstructures of composite materials efficiently. By leveraging the power of machine learning algorithms, the project seeks to predict material properties based on the generated synthetic microstructures. The overall flow of the project can be visualized in the following diagram.



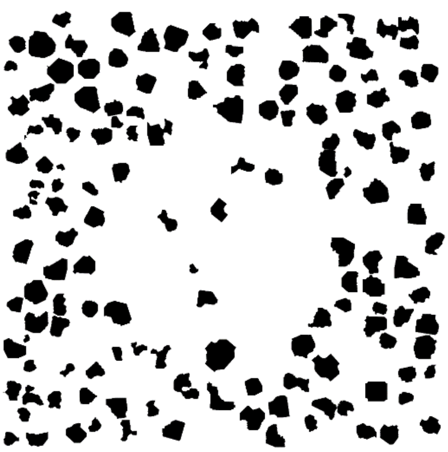
Overall Workflow of the Project

The project begins with the utilization of the FEniCS framework, a powerful computational toolkit for solving partial differential equations, to perform finite element method (FEM) simulations. These simulations generate property plots, such as stress intensity and displacement patterns, for composite materials under different conditions. These property plots serve as labeled data for training a Generative Adversarial Network (GAN) model. The GAN model is designed to learn from the labeled data and generate synthetic microstructures that closely resemble real microstructures obtained from the FEM simulations. The generator network of the GAN produces synthetic microstructures, while the discriminator network evaluates the authenticity of these generated samples. Through an adversarial training process, the generator improves its ability to generate microstructures that accurately represent the properties observed in the FEM simulations. Once the GAN model is trained, it can be used to predict stress intensity and displacement patterns for unseen microstructures. This prediction capability provides a powerful tool for materials engineers to explore and analyze the mechanical properties of composite materials without relying solely on physical experiments. The outcomes of this research project demonstrate the potential of GAN models in accurately predicting material properties based on synthetic microstructures. This approach opens up new avenues for materials engineering, offering a more efficient and cost-effective way to generate and analyze microstructures. By combining image processing, computational modeling, and machine learning, researchers can gain a deeper understanding of composite materials and design them with tailored mechanical properties. In conclusion, this project represents a significant step forward in materials engineering by leveraging the power of synthetic microstructure generation and machine learning. The integration of image processing, computational modeling, and ML techniques offers a novel approach to predict material properties and accelerate the development of advanced composite materials.

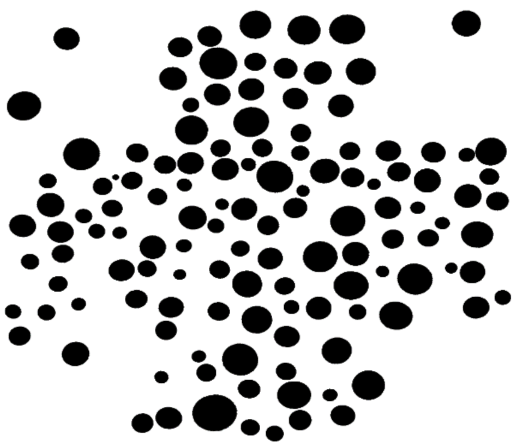
Methodology

1.Generation of Synthetic Dataset of Microstructures

The methodology employed for generating the dataset of synthetic microstructures with circular and irregular grains involved a systematic and comprehensive approach. A total of 360 images were generated, encompassing various combinations of distributions, sizes, area fractions, and random placements. To begin, four different distributions—homogeneous, plus, hyperbolic, and circular—were implemented using Python. These distributions were selected to capture different grain arrangements and spatial patterns within the microstructures. The distributions served as the basis for generating microstructures with both circular and irregular grains. Next, three different size variations—single mode, Gaussian, and bimodal—were introduced to the microstructures. These size variations were applied to both circular and irregular grains, resulting in a diverse range of grain sizes within the dataset. This variation in grain sizes allowed for the exploration of size-dependent phenomena and the analysis of size-structure relationships. To further enhance the diversity of the dataset, three different area fractions were considered for each combination of distribution and size variation. This led to a total of 36 distinct variations of microstructures for both circular and irregular grain shapes. The inclusion of different area fractions enabled the study of the influence of grain density on material properties and behaviour. To ensure the uniqueness of each microstructure, a random placement algorithm was implemented. By randomly placing the grains within the microstructure domain for each combination, five different microstructures were generated. This randomized placement accounted for the stochastic nature of grain arrangement, resulting in varied and representative microstructure samples. Overall, this methodology produced a comprehensive dataset of 180 microstructures with circular and irregular grains. The combination of different distributions, size variations, area fractions, and randomized placements allowed for a wide range of microstructure samples. This dataset provides valuable resources for studying microstructure-property relationships, developing models, and validating algorithms in the field of materials science and engineering.



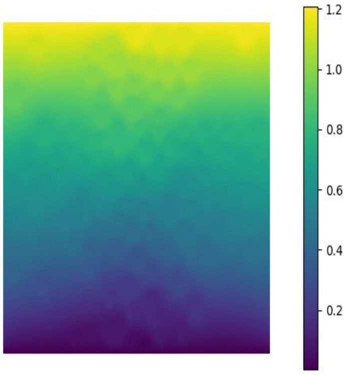
Irregular Shaped with circular distribution Microstructure



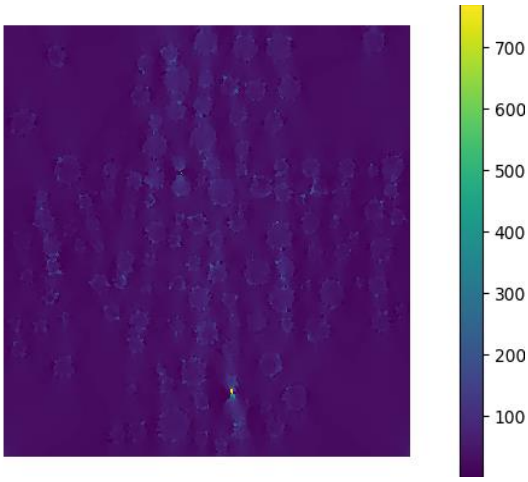
Circular Shaped with plus distribution Microstructure

2.Generating dataset by use of FEniCS for FEM Analysis

In addition to generating the dataset of synthetic microstructures, Finite Element Method (FEM) simulations were conducted to obtain property plots for each microstructure. The two properties of interest were stress intensity and displacement, which were simulated and visualized to gain insights into the mechanical behavior of the microstructures. For each microstructure in the dataset, FEM simulations were performed using appropriate boundary conditions and loading scenarios. The simulations were run using established software packages capable of solving the governing equations of solid mechanics and generating property plots. The stress intensity plots provided a visualization of the distribution and magnitude of stress within the microstructures. This information is crucial for understanding the stress concentration, areas of potential failure, and the overall structural integrity of the materials. By analyzing the stress intensity plots, researchers can gain valuable insights into the mechanical response of the microstructures under various loading conditions. Similarly, the displacement plots were generated to illustrate the deformations and displacements experienced by the microstructures. These plots depicted the magnitude and direction of displacements at different points within the material. This information is important for assessing the structural stability, deformation patterns, and potential areas of strain accumulation within the microstructures. The property plots obtained from the FEM simulations served as the target outputs for the Machine Learning (ML) model developed in this study. The input to the ML model was the microstructure images, and the corresponding stress intensity and displacement plots were used as the ground truth for training and evaluation. By training the ML model using the dataset of 180 microstructures with their corresponding property plots, the model learned to establish a relationship between the microstructure images and the desired property plots. This ML model could then be used to predict property plots for unseen microstructures, providing a fast and efficient means of analyzing the mechanical behavior of complex microstructures. Overall, the methodology encompassed conducting FEM simulations to generate stress intensity and displacement plots for the entire dataset of 180 microstructures. These property plots served as the target outputs for training an ML model, which could then be utilized for predicting property plots based on microstructure images. This integrated approach allowed for a comprehensive analysis of the mechanical properties of the synthetic microstructures and facilitated the development of a predictive tool for future microstructure-property investigations.



FEniCS Generated Displacement Plot



FEniCS Generated Stress Intensity Plot

3.Machine Learning for prediction

The image-to-image translation task in this study was accomplished using a pix2pix Generative Adversarial Network (GAN) model. The GAN consisted of two main components: the generator and the discriminator. The GAN was trained for 50, 100, 150, 200, and 250 iterations to optimize the translation process.

1.Generator

The generator played a pivotal role in the pix2pix GAN model. It was responsible for transforming the input microstructure images into property plots. The generator utilized a U-Net architecture, a commonly used deep learning model for image translation tasks. The U-Net architecture consisted of an encoder-decoder structure, where the encoder portion learned the features from the input images and the decoder portion generated the corresponding property plots. The generator was trained to generate property plots that closely resembled the ground truth obtained from the FEM simulations. It was trained using a combination of an adversarial loss, which encouraged the generator to produce realistic property plots, and a pixel-wise loss, which enforced pixel-level similarity between the generated and ground truth property plots.

2.Discriminator

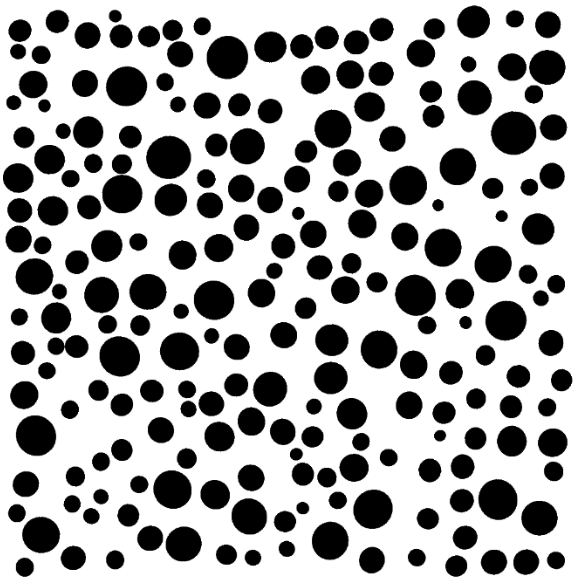
The discriminator played a critical role in training the generator. Its purpose was to distinguish between the generated property plots and the ground truth ones. A Patch GAN was used in this regard. The discriminator had a convolutional neural network (CNN) architecture that learned to classify the input images as either real (ground truth property plots) or fake (generated property plots). By providing feedback to the generator based on its classification, the discriminator guided the generator towards producing more realistic and accurate property plots. The discriminator loss was calculated based on the accuracy of its classification and was used to update the weights of the discriminator during training.

Throughout the training process, the generator and discriminator were engaged in a competitive game. The generator aimed to generate property plots that could fool the discriminator into classifying them as real, while the discriminator aimed to accurately classify the real and fake property plots. This adversarial training process encouraged the generator to improve its output quality over time. The GAN model was trained for multiple iterations, including 50, 100, 150, 200, and 250 iterations, to optimize the translation performance. The number of iterations was determined based on the convergence of the loss functions and the visual quality of the generated property plots. Increasing the number of iterations allowed for a more refined and accurate translation from microstructure images to property plots. In summary, the pix2pix GAN model employed in this study consisted of a generator and a discriminator. The generator utilized a U-Net architecture to transform microstructure images into property plots, while the discriminator learned to differentiate between real and generated property plots. Through adversarial training, the generator improved its translation performance over multiple iterations.

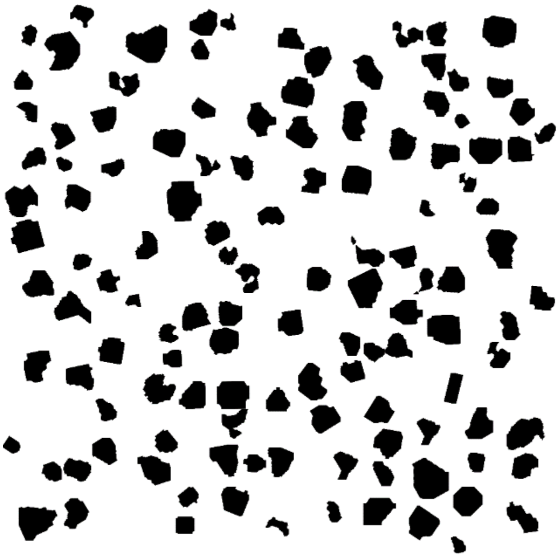
Results

The results of the study revealed the creation of two distinct datasets, each focusing on different types of microstructures: circular grains and irregular grains. These datasets were generated with careful consideration of various parameters, resulting in a diverse range of microstructure samples. In the first dataset, circular grains were chosen as the primary shape. A systematic variation of parameters such as size, distribution, orientation, and area fractions was applied to ensure a wide range of microstructure variations. By systematically manipulating these parameters, the dataset was able to capture the diversity of circular grain microstructures commonly encountered in materials. The second dataset focused on irregular grains, which deviated from the uniformity of circular grains. This dataset aimed to represent more complex and realistic microstructure configurations. The irregular grain shapes introduced additional complexity and diversity, providing a broader representation of real-world materials.

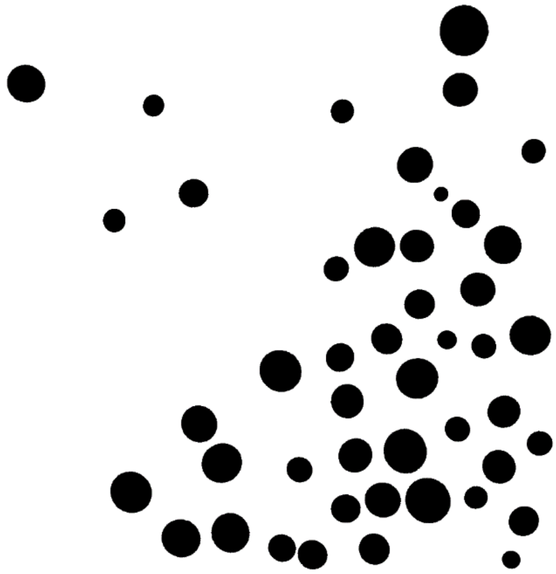
Irregular Shaped with plus distribution Microstructure



Circular Shaped with homogenous distribution Microstructure

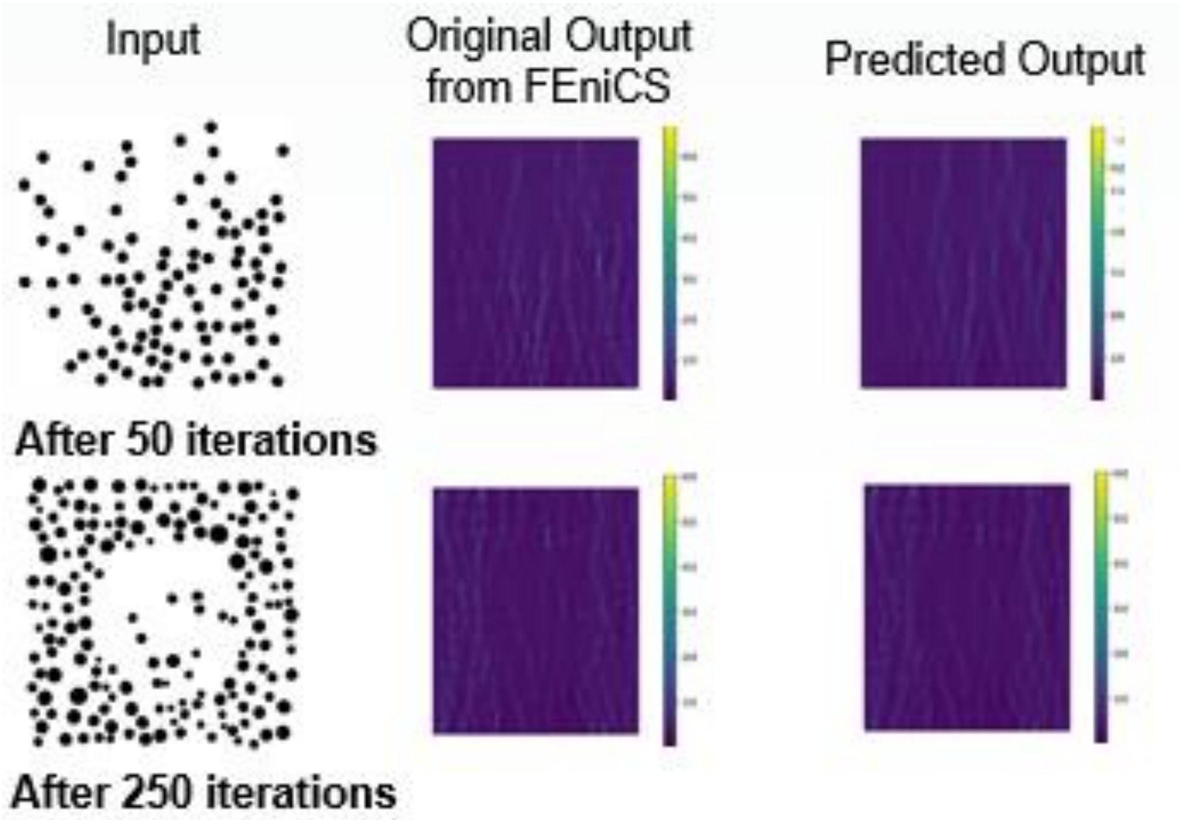


Irregular Shaped with homogeneous distribution Microstructure

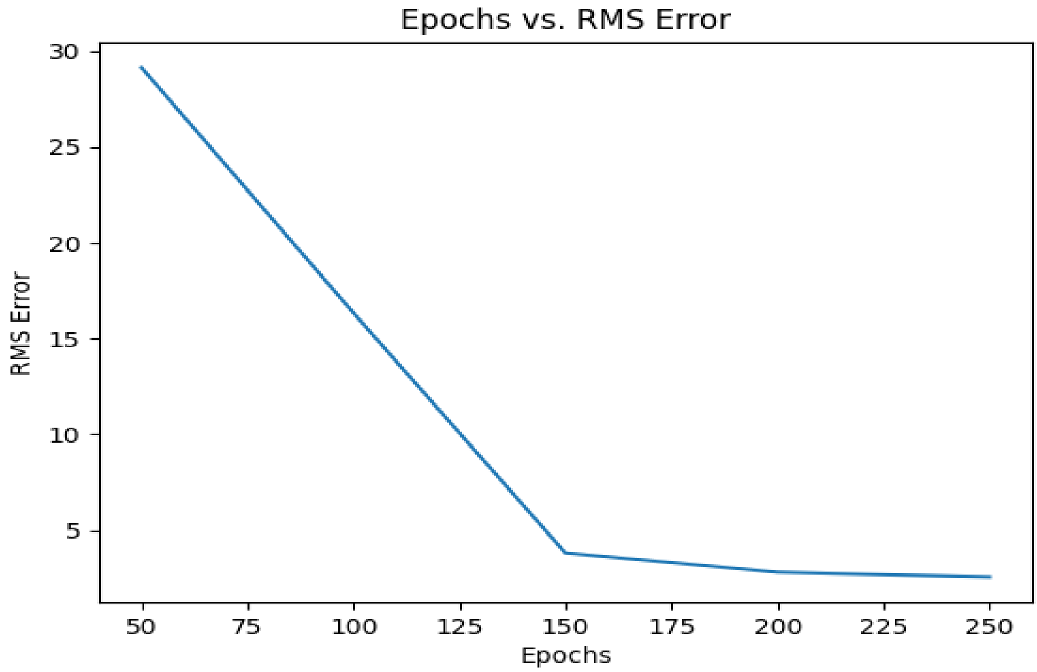


Circular Shaped with hyperbolic distribution Microstructure

The GAN model was trained on various iterations, and the results are shown below.



This diagram showed that the model performed really well after 250 iterations as compared to 50 iterations. Below is a graph showing RMS Error vs Iterations showing that the error reduces drastically.



The graph visually depicts the relationship between the number of iterations and the corresponding RMS error, showcasing the reduction in error with increased iterations.

Conclusion

We have presented the successful generation of synthetic microstructures using Generative Adversarial Network (GAN) models. This achievement has allowed us to create a comprehensive dataset containing microstructure images and corresponding stress intensity images. By leveraging the power of Machine Learning, we have developed a framework that can accurately predict the stress intensity of a two-phase composite microstructure image. The application of GAN models for generating synthetic microstructures and predicting their properties has significant implications for the understanding and design of composite materials. Traditionally, obtaining microstructure properties involved time-consuming and expensive physical experimentation. However, our developed framework offers an alternative approach that overcomes these limitations. By harnessing the capabilities of GAN models, we can now generate a vast range of synthetic microstructures that closely resemble real-world samples. These synthetic microstructures, along with their associated stress intensity images, provide a valuable resource for training and testing Machine Learning models. Through extensive experimentation and optimization, our framework has demonstrated impressive accuracy in predicting stress intensity based on microstructure images. The ability to predict microstructure properties through Machine Learning models has wide-ranging implications. It enables researchers and engineers to explore and understand the behavior of composite materials in a virtual environment, saving significant time and resources. Moreover, the framework opens avenues for accelerated material design and optimization processes, as the properties of various microstructures can be assessed rapidly without physical fabrication and testing. Our results highlight the potential of GAN models in predicting microstructure properties and their contribution to advancing the field of composite materials. However, it is essential to acknowledge the limitations and areas for further improvement. The accuracy of the predictions relies on the quality and diversity of the dataset, as well as the design of the GAN architecture. Continual refinement of the dataset and exploration of advanced GAN variations can enhance the performance and generalization of the predictive models. In conclusion, the development of a framework combining GAN models and Machine Learning techniques has demonstrated the ability to predict stress intensity from two-phase composite microstructure images. This approach offers a promising alternative to traditional physical experimentation for obtaining microstructure properties. The generated dataset and the predictive models contribute to the understanding, design, and optimization of composite materials, enabling researchers and engineers to make informed decisions and accelerate the development process. This research paves the way for further advancements in the application of GAN models in materials science and opens new possibilities for virtual exploration and design in the field of composite materials.

Future Work

The project's next step is to train the model to generate the Displacement Plot for circular-shaped microstructures. Further, we will develop a similar dataset for the microstructure containing irregularly shaped grains in future.

References and Acknowledgment

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