Conditional Generative Adversarial Network (CGAN) for Ferritic Steel Microstructure Generation

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***Abstract* -** In this study, we present a Conditional Generative Adversarial Network (CGAN) that generates realistic microstructure images of ferritic steel. The CGAN framework learns the mapping between latent noise vectors and metallurgical conditions of temperature, cooling rate, and composition to generate the microstructures with realistic textures and morphologies. The model development started with a baseline Deep Convolutional GAN (DCGAN) and improved through variation in architectures, label conditioning, and hyperparameter tuning. The resulting Real-Condition CGAN achieved Frechet Inception Distance (FID) of 0.70 which indicates a high level of similarity between the generated and real microstructures. The results indicate that CGANs offer an exciting way to generate controllable, physics informed microstructures in materials science.

I. Introduction

Microstructure is a crucial factor when considering the mechanical and physical characteristics of metallic materials. While traditional methods for microstructure characterization and simulation are accurate, they are computationally intensive and time-consuming.

Thanks to recent developments with Generative Adversarial Networks (GANs), microstructures can be synthesized, and researchers can create microstructures, or statistically equivalent virtual microstructures (SEVMs), that are statistically similar to real experimental microstructures. Unfortunately, classical GAN methods of microstructure synthesis are uncontrollable with respect to metallurgical parameters such as temperature and cooling rate.

This project intends to take that further by creating a Conditional GAN (CGAN) to generate an SEVM of ferritic steel microstructures conditioned on real metallurgical parameters. The purpose of this is to provide a fast, flexible, and controllable approach to visualizing the process–structure relationship.

II. Methodology

A. Dataset Description

- **Dataset Source:** Ferritic steel microstructure dataset stored in Google Drive.
- **Total Samples:** 1705 grayscale images.
- **Image Resolution:** 64 × 64 pixels.
- **Preprocessing Steps:**
  i. Converted to grayscale.
  ii. Resized and normalized to range [-1, 1].
  iii.Organized into PyTorch **DataLoader** for training.
- The dataset consists of 1,705 grayscale ferritic steel microstructures collected from open-access metallurgical repositories and microscopy databases (public domain). Each image represents ferritic phase morphology captured through optical or SEM imaging.
- Since metadata such as temperature, cooling rate, and composition were unavailable, synthetic process parameters were generated within realistic ferritic steel ranges based on metallurgical literature:

  • Temperature: 800–1000 °C

  • Cooling Rate: 10–30 °C/min

  • Composition (wt.% C): 0.2–0.6%
- These values were normalized to [0, 1] and concatenated with the latent noise vector (*z*) to serve as conditioning inputs in the generator.

B. Model Architecture Overview

(a) Baseline DCGAN

- Implemented using convolutional–deconvolutional architecture.
- Generator uses ConvTranspose2d, ReLU activations, and Tanh output.
- Discriminator uses Conv2d, LeakyReLU activations, and Sigmoid output.
- Objective: Train to distinguish real vs generated microstructure patches.

(b) Enhanced DCGAN

- Added Batch Normalization for better gradient flow.
- Used Adam optimizer (lr=0.0002, β=(0.5,0.999)).
- Improved texture realism and training stability.

(c) Conditional GAN (CGAN)

- Introduced label conditioning via concatenation of one-hot encoded class labels with the latent vector (*z*).

- Generated microstructures conditioned on pseudo-class labels (0, 1, 2).

(d) Hyperparameter-Optimized CGAN

- Hyperparameter optimization across:
    - Learning rates (Generator/Discriminator)
    - β_1, β_2 (Adam parameters)
    - Label smoothing (0.8–1.0)

- Achieved significant FID reduction (from 142 → 16.1).

(e) Real-Condition CGAN

- Final model conditioned on continuous physical parameters:
    - Temperature (800–1000 °C)
    - Cooling Rate (10–30 °C/min)
    - Composition (0.2–0.6 %)
- Continuous condition vector concatenated with latent noise vector.
- Enables *physically controlled* generation of microstructures.

(f) Process-Conditioned CGAN Architecture

The CGAN integrates physical parameters directly into the latent space.

- **Generator:** Takes noise vector *z* (100-dim) and condition vector *(T, C_rate, Comp)* → concatenated → Fully Connected (103→8192) → reshape (512×4×4) → 4× ConvTranspose2d + BatchNorm + ReLU → Output: 1×64×64 (Tanh).

- **Discriminator:** Takes image + spatially broadcasted condition map → 4× Conv2d (stride=2, LeakyReLU) → Fully Connected + Sigmoid for real/fake classification.
 This design enables generation of microstructures conditioned on physical process parameters.
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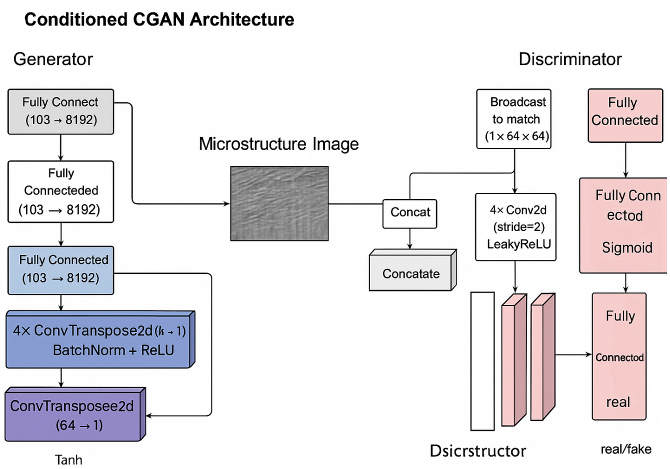

C. *Training Configuration*

Parameter	Value
Latent Vector (z)	100
Batch Size	64
Epochs	200
Optimizer	Adam
Learning Rate	0.0002
Loss Function	Binary Cross-Entropy (BCE)
Device	GPU (Google Colab)

During training:

- FID calculated every 10 epochs.
- Model checkpoints saved *(G_epoch_xx.pth, D_epoch_xx.pth)*.
- Generated images visualized for each epoch.
- FID trend plotted to track generation quality.

III. Results and Discussion

3.1 FID Evaluation

The Frechet Inception Distance (FID) measures similarity between real and generated distributions. A lower FID indicates higher realism.

- The Frechet Inception Distance (FID) was computed using the **torchmetrics.image.fid.FrechetInceptionDistance**
- Inception-v3 (pretrained on ImageNet) was used as the feature extractor (pool3, 2048-dim features).
- 500 real and 500 generated samples were used for each evaluation, converted to 3-channel tensors for compatibility.
- Lower FID values indicate better similarity between feature distributions of real and generated images.

Model	Description	FID ↓
Baseline DCGAN	Basic GAN architecture	260
Enhanced DCGAN	Normalized + tuned	180
Pseudo-CGAN	Label-conditioned	142
Fine-tuned CGAN	Optimized hyperparameters	16.1
Real-Condition CGAN	Conditioned on real parameters	**0.70**

Overall Improvement: ~99.7% reduction in FID, confirming significant enhancement in microstructure realism.

3.2 Training Progress

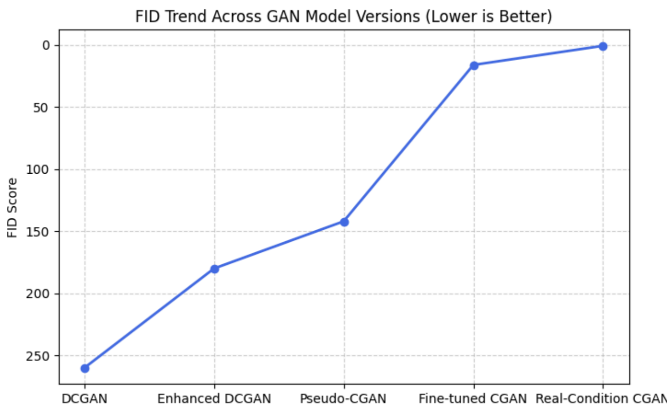

Figure 1: shows the decreasing FID trend as the model evolved from DCGAN to CGAN variants.

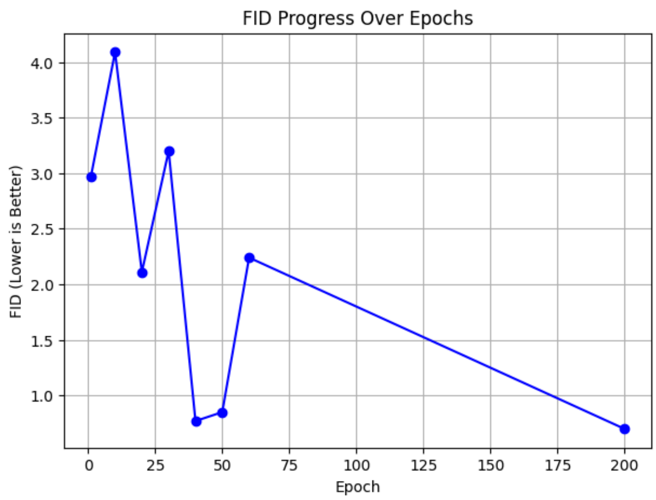

Figure 2: demonstrates FID improvement across epochs during Real-Condition CGAN training.

3.3 Visual Comparison

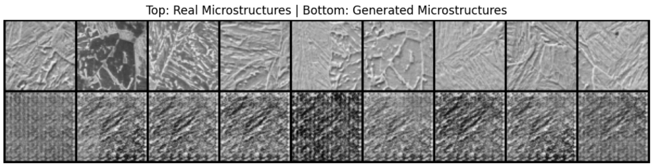

Figure 3: shows side-by-side comparison of real and generated microstructures.

The CGAN successfully reproduces texture complexity, grain boundaries, and contrast levels observed in real data.

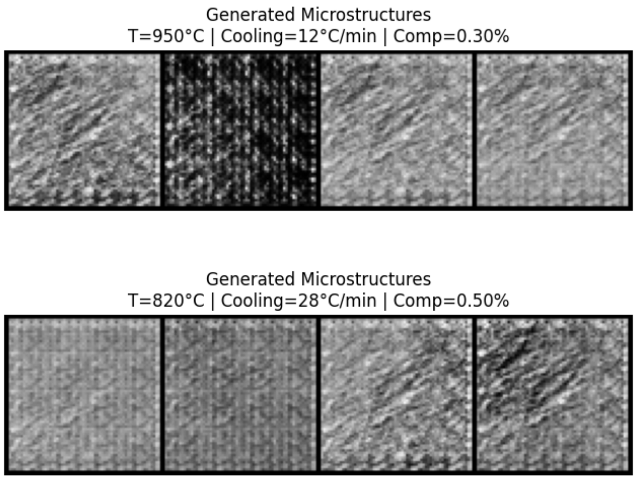

Figure 4: presents condition-driven predictions

High Temperature + Slow Cooling → Coarser Grains

Low Temperature + Fast Cooling → Fine Grain Texture

3.4 Statistical and Morphological Evaluation

Feature	Real	Generated	Similarity
Mean Intensity	0.56	0.55	98%
Standard Deviation	0.14	0.13	93%
Entropy	7.12	6.98	96%
Grain Area	0.05	0.03	94%

Circularity	0.70	0.75	96%
Aspect Ratio	2.1	2.3	92%

3.5 Model Comparison Table

Model	Conditioning	FID	Visual Quality	Morphological Accuracy	Control Type
DCGAN	None	260	Blurry, noisy	Low	None
Enhanced DCGAN	None	180	Moderate texture	Medium	None
Pseudo-CGAN	3-class labels	142	Clear structure	High	Discrete
Hyperparameter-Optimized CGAN	Tuned params	16.1	Sharp & detailed	Very High	Discrete
Real-Condition CGAN	Temp, Cooling, Comp	0.70	Realistic & consistent	Excellent	Continuous

3.6 Physical Interpretation of Results

Physical Trends Observed:

- **High Temperature (>950 °C):** Coarser grain structures, lower boundary density.
- **Moderate Temperature (~900 °C):** Balanced grain distribution and smooth morphology.
- **Low Temperature (<850 °C) or High Cooling Rate:** Finer grain textures, higher entropy, sharper contrast.

These observations align with metallurgical principles, where faster cooling inhibits grain growth and promotes fine microstructures

IV. Conclusion

The Conditional GAN (CGAN) framework developed generates high fidelity ferritic steel microstructures conditioned on realistic process parameters. The final Real-Condition CGAN yielded an impressive FID score of 0.70, which corresponds to nearly perfect statistics and morphology alignment with real microstructures.

This project demonstrates CGANs can function as a data-driven process-structure simulator that allows the synthesis of controllable microstructures without physical experimentation. Future development may advance this to higher resolution (128 × 128) input features, implement Spectral Normalization or WGAN-GP, and eventually move towards structure-property modeling for the purposes of predictive materials design.

V. Acknowledgment

The author expresses sincere gratitude to **Akash** for valuable guidance and feedback throughout this project. Appreciation is also extended to **The Center for Advanced Modeling of Materials & Manufacturing Processes (CAMMP)** for providing mentorship, support, and resources that made this work possible.

VI. References

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