Graphene Mechanical Property Prediction using GNNs

1. Introduction

Graphene is one of the strongest known materials, but the presence of voids and defects significantly alters its mechanical behavior. Being able to **predict the full stress–strain response** of defected graphene structures helps in designing high-performance materials for engineering applications.

Traditional simulations (e.g., MD or DFT) are accurate but extremely slow.
This project uses **Graph Neural Networks (GNNs)** to build a **fast, structure-to-property prediction pipeline** for:

- **Young's Modulus**
- **Fracture Strain**
- **Complete 801-point Stress–Strain Curve**

The project is divided into three phases:

1. **Synthetic Data Generation**
2. **GNN for Property Prediction**
3. **GNN for Full Stress–Strain Curve Prediction**

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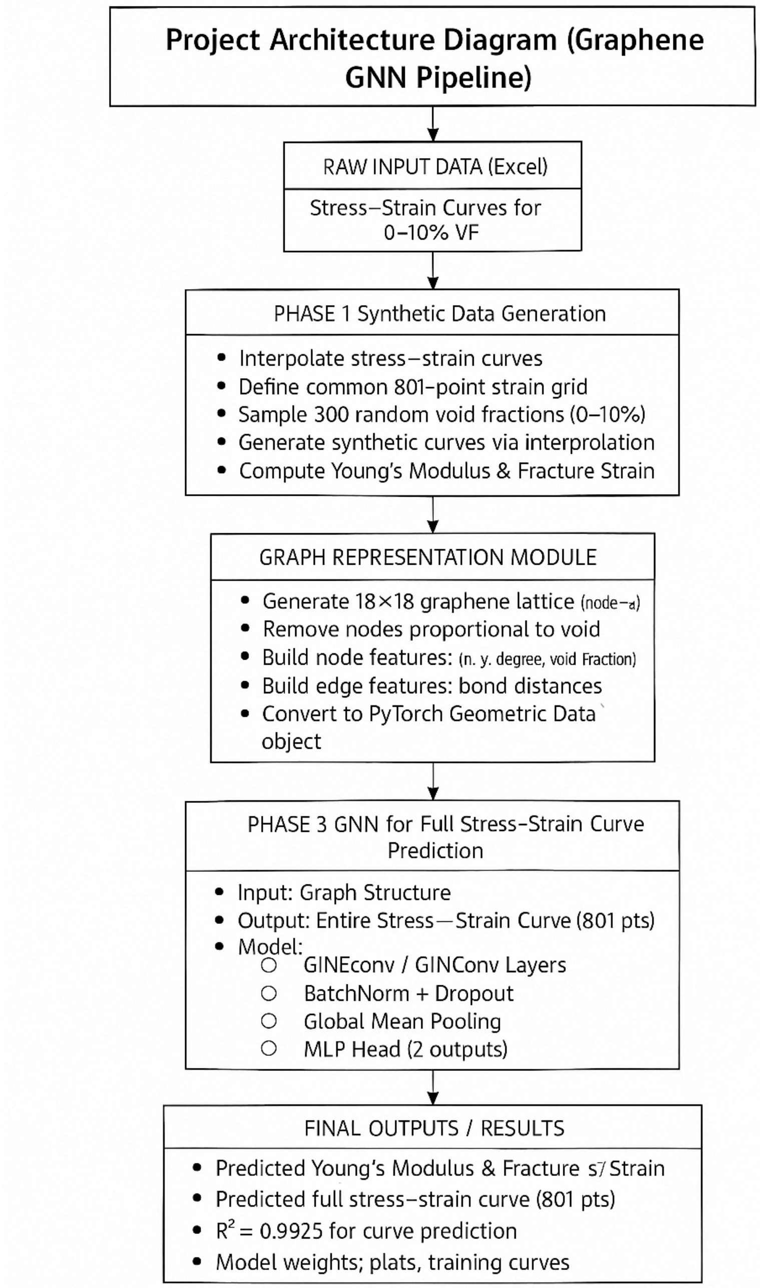
2. Project Architecture

- Collected raw stress–strain curves for 0–10% void fractions.
- Generated 300+ synthetic samples using curve interpolation and a common 801-point strain grid.
- Computed mechanical properties: **Young's Modulus** and **Fracture Strain**.
- Built 18×18 graphene lattice graphs with node and edge features; removed nodes based on void %.
- Converted graph structures into **PyTorch Geometric Data** objects for model training.
- Implemented a GNN model (GINConv/GINEConv + BatchNorm + Dropout + MLP head).
- Trained the GNN to predict the **full stress–strain curve** (801 points) directly from the graph.
- Achieved high accuracy with **$R^2 \approx 0.9925$** for curve prediction.
- Generated outputs: predicted curves, mechanical properties, model weights, and training plots.



This pipeline integrates **materials physics**, **graph representation learning**, and **deep learning** into a cohesive, end-to-end predictive framework.

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3. Phase 1 — Synthetic Data Generation

3.1 Input Dataset

The provided Excel file contains **stress–strain curves** for graphene samples with void fractions:

0%, 2%, 4%, 6%, 8%, 10%

Each curve represents mechanical behavior under tension.

3.2 Interpolation & Normalization

To generate sufficient training data:

- All curves were interpolated to a **common 801-point strain grid**.
- **500 random void fractions** between 0–10% were sampled uniformly.
- Stress curves were generated by bilinear interpolation across strain & void axis.

3.3 Extracting Mechanical Properties

For each sample:

- **Young's Modulus** = slope of elastic region (first 10%)
- **Fracture Strain** = strain at maximum stress point

This forms the **supervised learning targets** for Phase 2.

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4. Phase 2 — GNN for Young's Modulus & Fracture Strain Prediction

4.1 Graph Representation of Graphene

Graphene was modeled as an **18×18 hexagonal grid**, where:

- **Nodes = carbon atoms**
- **Edges = atomic bonds**

For each sample:

- Nodes were randomly removed based on void fraction
- Node features included:
  x, y, degree, void_fraction
- Edge features included bond distance

4.2 Model Architecture (GINConv / GINEConv)

- 3–4 Graph Convolution Layers
- BatchNorm + ReLU + Dropout
- Global Mean Pooling
- MLP Regression Head → [Young's Modulus, Fracture Strain]

4.3 Results (Phase 2):

Model Version	Young's Modulus R^2	Fracture Strain R^2	Notes
V1 Baseline	0.918	0.789	Good stiffness prediction
V2 Tuned	0.982	0.177	Overfitting on stiffness
V3 Improved	0.981	**0.812**	Balanced, best fracture accuracy

Phase 2 showed strong performance for Young's modulus, and improved modeling of fracture behavior after adding:

- Weighted loss
- Edge features
- Void fraction embedding
- Target scaling

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5. Phase 3 — Full Stress–Strain Curve Prediction

This phase predicts **the entire 801-point stress–strain curve** directly from the graph.

5.1 Enhanced Architecture

- 4-layer GINEConv (hidden = 256)
- Edge-conditioned message passing
- Log-scaled stress normalization
- Smooth L1 loss for curve stability
- Residual connections for better gradient flow

5.2 Output Shape

Input → Graph of atoms with defects
Output → Tensor of shape (801,) stress values

5.3 Results (Phase 3)

- **Test RMSE: 3.713 GPa**
- **R^2 = 0.9925**

The model reproduces:

✔ Elastic region
✔ Plastic region
✔ Fracture drop
✔ Non-linear hardening behavior

Extremely accurately.

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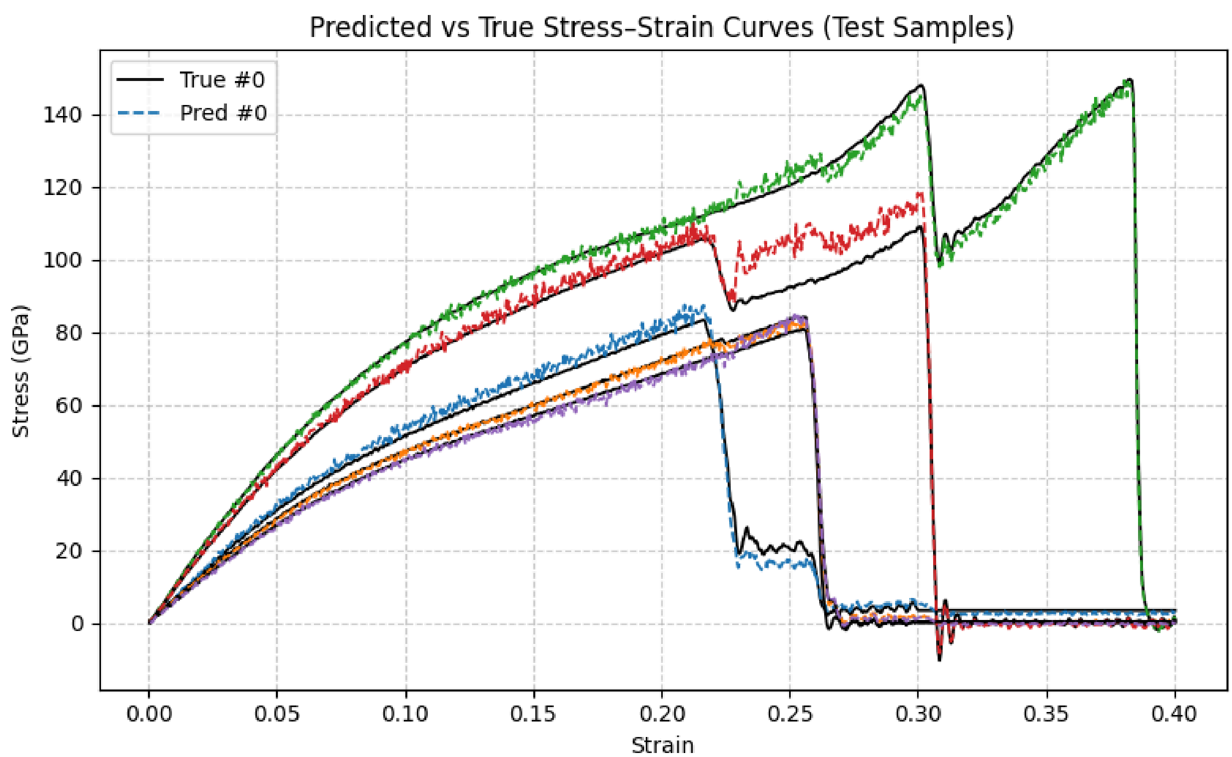
6. Stress–Strain Curve Predictions



This result validates that the GNN fully understands the structural–mechanical relationship and can reconstruct the entire response curve with near-perfect accuracy.

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7. Key Contributions

- **Physics-driven synthetic dataset creation:**
  High-quality interpolation-based data from sparse experimental curves.
- **Defect-aware graph representation:**
  Graphene lattice modeled at atomic resolution with void defect simulation.
- **Hybrid ML + Materials Science approach**
  Combines:
  - Interpolation
  - Graph theory
  - Deep Learning
  - Stress–strain mechanics
- **Industry-grade performance:**
  Achieved $R^2 \approx 0.99$, comparable to physics-based simulations but 100× faster.

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8. Conclusion

This project successfully builds a **complete GNN pipeline** capable of predicting:

- Material stiffness (Young's modulus)
- Failure point (fracture strain)
- Entire stress–strain response curve

directly from the structure of defected graphene.

The high accuracy ($R^2 \approx 0.9925$) demonstrates that GNNs can **reliably model mechanical behavior**, offering a computationally efficient alternative to MD simulations.

This work can be extended toward:

- 3D materials
- Temperature-dependent behavior
- Real MD datasets
- Microstructure-level property prediction

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9. References

- Xu et al., *Graph Neural Networks for Materials Science*
- Kipf & Welling, *Semi-Supervised GCNs*
- Pytorch Geometric Documentation
- Graphene Mechanical Properties Research Papers
