COLUMBIA ENGINEERING

Deep Learning Loss Function and Data Optimization for A.I. Detection of Thin Film Grain Boundaries

COLUMBIA NANO INITIATIVE

National Science Foundation

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Background

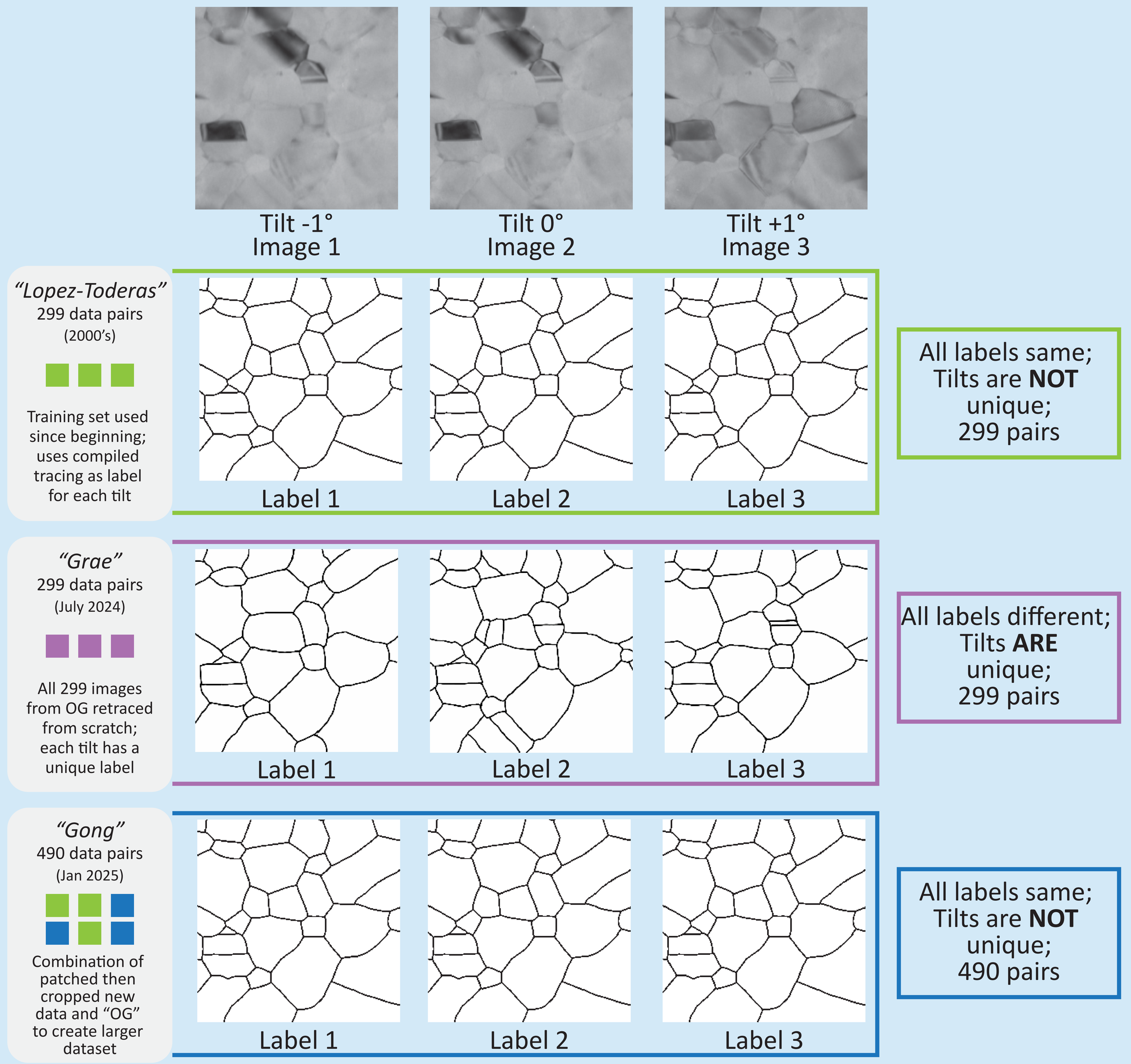
- Understanding microstructural features of materials is essential for predicting materials' properties.
- Grain boundaries significantly influence mechanical strength, ductility, electrical resistivity, corrosion resistance, and thermal properties of metals and alloys.
- Tracing grain boundaries is crucial for determining the sizes of grains, but it is a labor-intensive, subjective task.
- A U-Net architecture [1], widely used in image segmentation, has shown promise for automated grain boundary tracing [2].
- Various loss functions can be employed to train and validate such a model, each potentially emphasizing different aspects of learning (e.g., boundary accuracy vs. robustness to data variability) [3].

Purpose

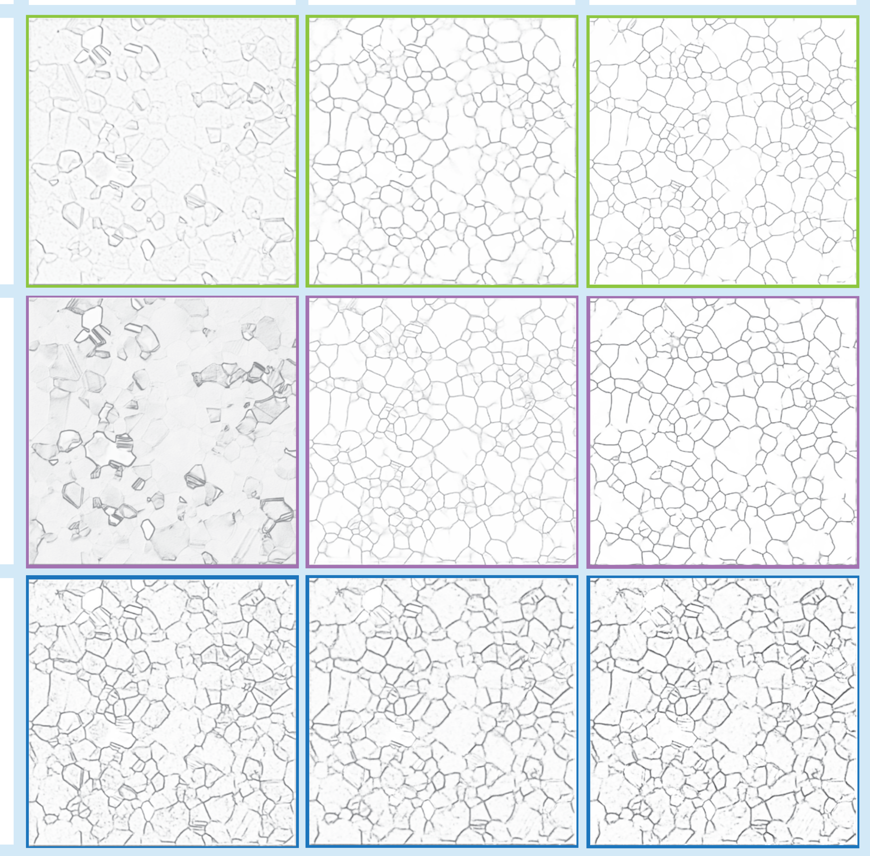
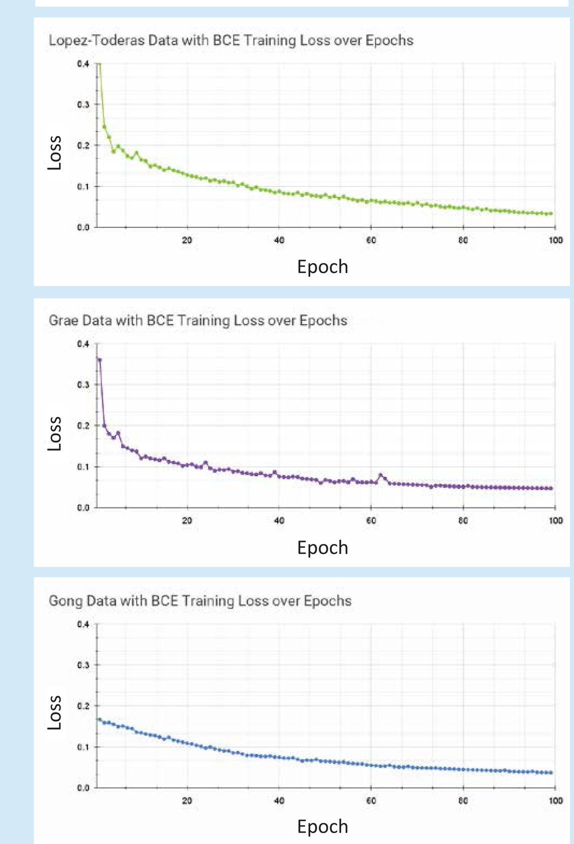
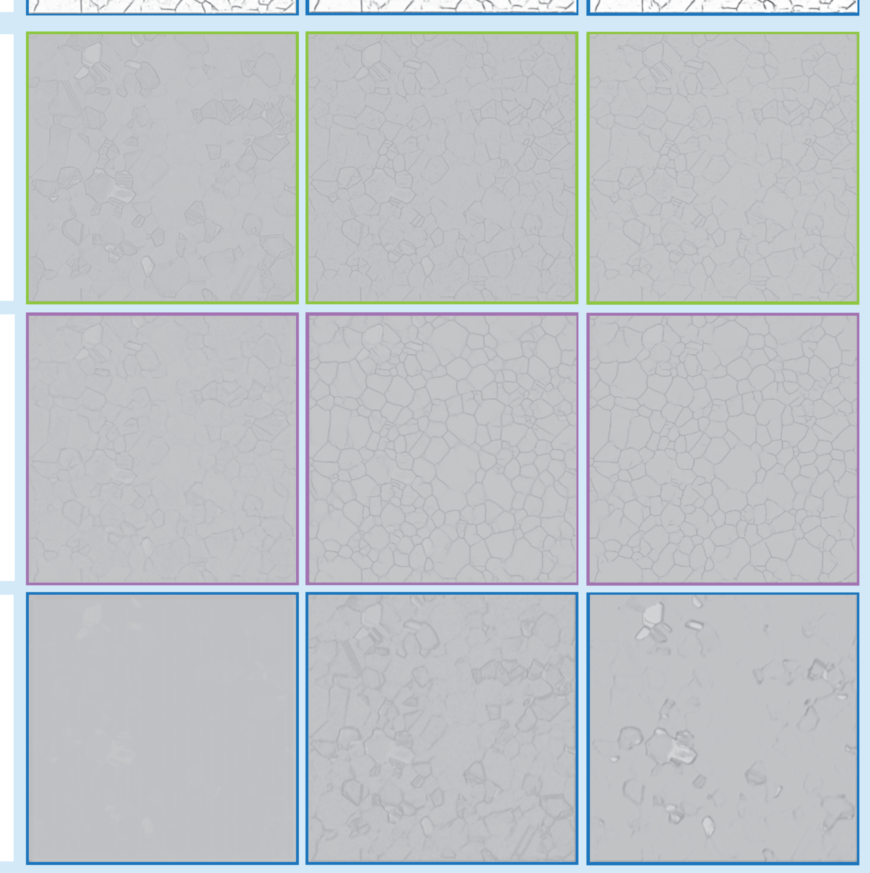
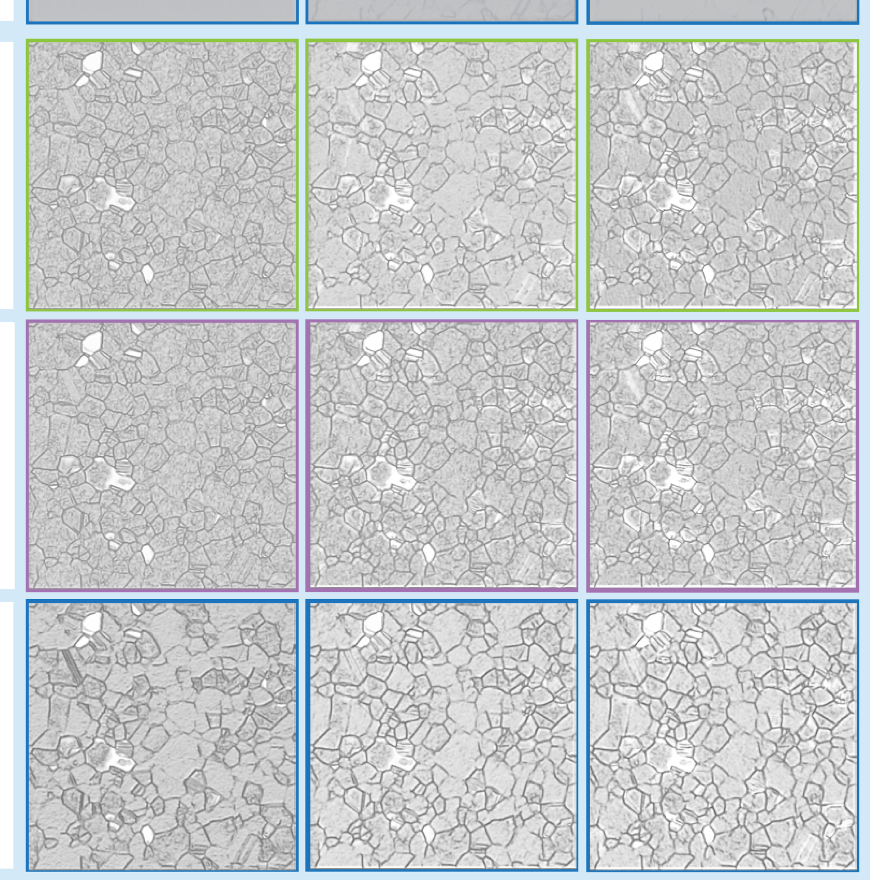
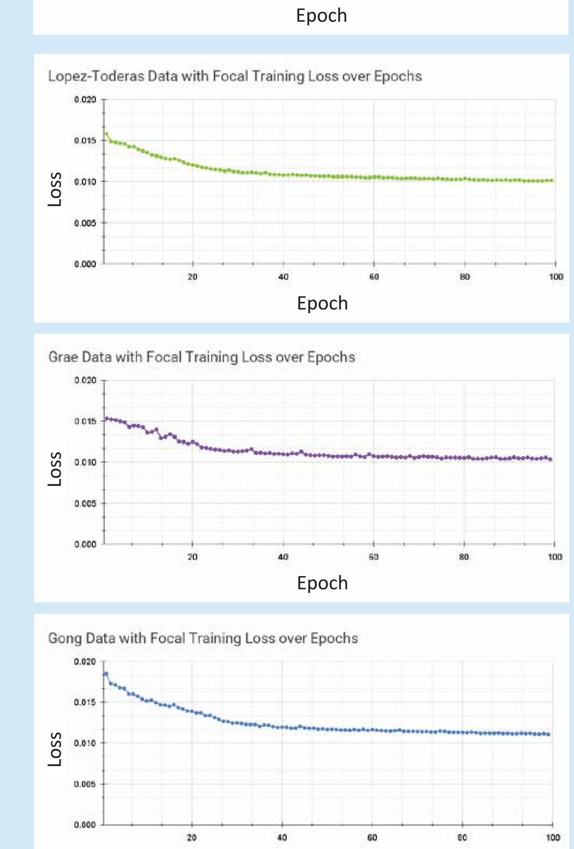
- **Identify optimal combination of loss function and data to create a model that can generates an automated tracing most consistent with the ground truth**
- **Explore if quality or quantity is more important for dataset construction when training a U-Net model.**

Methods

- Trained for 99 epochs using one of three built-in PyTorch loss functions, one of three prepared dataset (see below), ran inference test on on test image not in training set



Results

Loss Fn	Loss Function Formula and Purpose	Data set	24 Epochs	66 Epochs	99 Epochs	Training Loss
Binary Cross Entropy Loss	BCE Loss = $-\frac{1}{N}\sum_{i=1}^{N}[y_i \log(\hat{y}_i) + (1-y_i)\log(1-\hat{y}_i)]$ N: total number of pixels y_i: ground truth (1 if pixel belongs to grain boundary, 0 otherwise) $\hat{y}_i$: predicted probability of the pixel belonging to the grain boundary • BCE loss measures how well predicted probabilities align with actual binary ground truth labels • Predictions that deviate significantly from the true labels are strongly penalized	Lopez-Toderas Grae Gong				
Mean Squared Error Loss	MSE Loss = $\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$ N: total number of pixels y_i: ground truth (1 or 0, as above) $\hat{y}_i$: predicted probability for each pixel • Large prediction errors are penalized by squaring the difference between predicted probabilities and ground truth labels • Encourages the model to closely match pixel-wise predictions to ground truth	Lopez-Toderas Grae Gong				
Focal Loss	Focal Loss = $-\frac{1}{N}\sum_{i=1}^{N}[\alpha y_i(1-\hat{y}_i)^{\gamma}\log(\hat{y}_i) + (1-\alpha)(1-y_i)\hat{y}_i^{\gamma}\log(1-\hat{y}_i)]$ N: total number y_i: ground truth (1 or 0) $\hat{y}_i$: predicted probability for each pixel α: weighting factor for class imbalance (often 0.25 for positive class) γ: focusing parameter (typically set around 2) • Standard binary cross entropy loss is modified by down-weighting the contribution of well-classified examples and focusing more on difficult-to-classify pixels	Lopez-Toderas Grae Gong				

Conclusions

Loss Functions Analysis

- Can qualitativiely determine that BCE performs better than the other two loss functions given its closest visual resemblance to a tracing needed for post processing overlay applications

Datasets Analysis

- As expected, the Gong dataset experienced less loss with the model learning quicker from a larger dataset
- The Gong inference outputs appear to trace noise within the grains rather than their boundaries. This becomes most pronounced at 99 epochs indicating potential overfitting at earlier point in training than other two datasets
- Within the BCE results, the Grae dataset experienced more loss and has a larger minma than the Lopez-Toderas dataset; however, the Grae dataset is less prone to overfitting than the Lopez-Toderas dataset as per the train validation loss results
- Additionally, the Grae dataset is qualitatively superior
- At both 66 and 99 epochs Grae surpasses Lopez-Toderas in identifying smaller grains; Lopez-Toderas appears to output inferences with greater confidence at expense of complete tracing
- This indicates that a lesser quantity of higher quality data—for a U-Net architecture— out performs an equal or larger quantity of lower quality data in machine learning

Future Work

- Quantitative comparison of the methods using grain size distributions
- Experiment with more loss functions especially those not built into PyTorch
- Investigate if the construction of a fourth dataset with the same number of datum as Gong but created through the same approach as the Grae dataset will significantly improve model performance (quality and quantity)

References

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[2] Azad, R., Heidary, M., Yilmaz, K., Hüttemann, M., Karimijafarbigloo, S., Wu, Y., Schmeink, A., Merhof, D. (2023). Loss Functions in the Era of Semantic Segmentation: A Survey and Outlook. arXiv:2312.05391v1 [cs.CV] .

[3] Patrick, M., Eckstein, J., Lopez, J., Toderas, S., Asher, S., Whang, S., Levine, S., Rickman, J., Barmak, K.. (2023). Automated Grain Boundary Detection for Bright-Field Transmission Electron Microscopy Images via U-Net. Microscopy and Microanalysis. 29. 10.1093/micmic/ozad115.

Acknowledgements

Rosnel Leyva-Cortes, Jeffrey Rickman, Ralph Linares, Digna Linares

Partial funding support was provided by the U.S. National Science Foundation (NSF) under grant number DMS-1905492 and under the DMREF program under DMS-2118206. This work was carried out in part in the Electron Microscopy Laboratory of Columbia Nano Initiative (CNI) Shared Lab Facilities at Columbia University.