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MLDL

Machine Learning and Deep Learning Conference 2022

Utilization of the critic subnetwork of a generative adversarial network as detector of morphological material change in image data

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FY22 Exploratory Express LDRD, Project 226346

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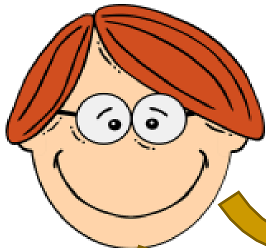
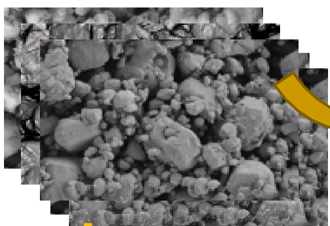
Problem

Surveillance

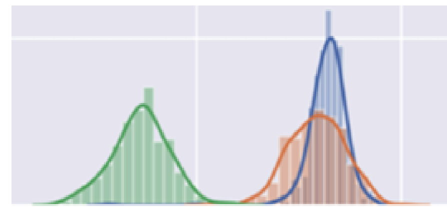




Segmentation

Dimensionality Reduction

Traditional morphology analysis



Single-point metrics
Spatial correlations
Regional statistics

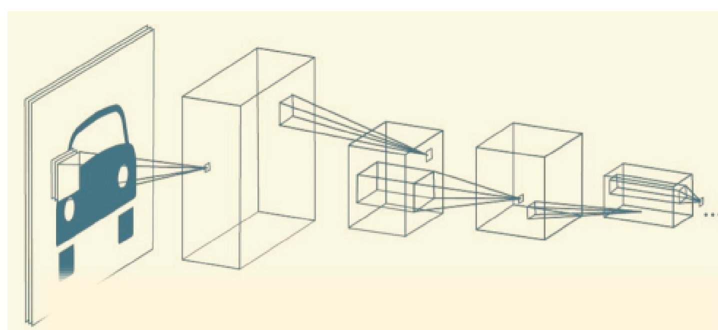
- A priori choice
- Information loss
- Dependence on experimental setup

Lack of test data

Original images

Representation of complex function

Computer Vision

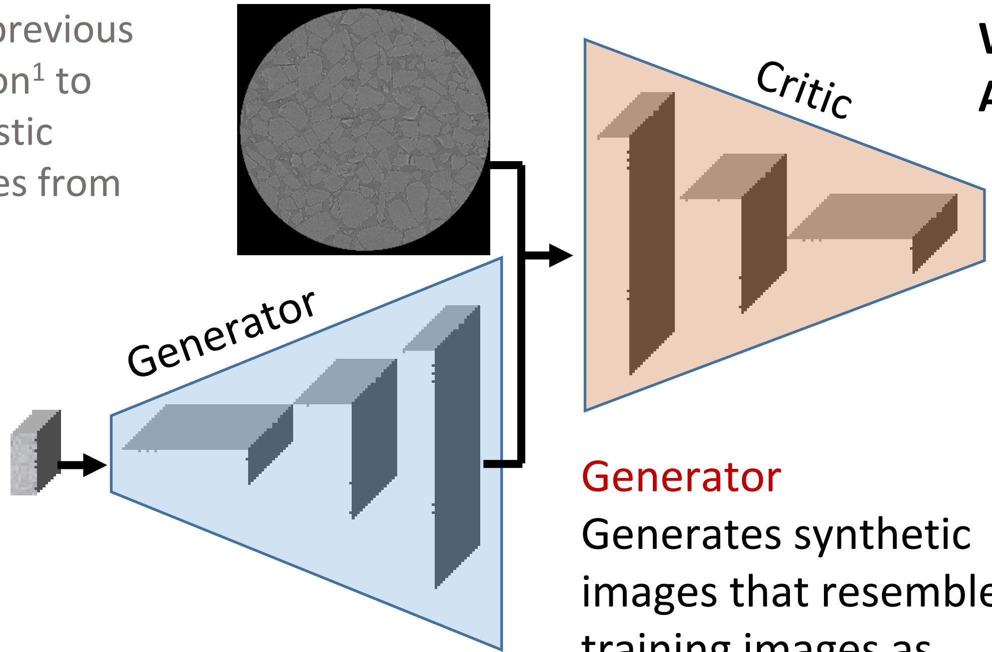


Convolutional neural network

- No prior choice
- Little information loss
- Reduced dependence on experimental setup

Algorithmic Approach

Utilization of previous implementation[1] to generate realistic microstructures from SEM images



Wasserstein Generative Adversarial Network (WGAN)

Critic
Scores generated images according to how well they resemble the training images

Generator
Generates synthetic images that resemble training images as closely as possible

Critic and generator **trained** together with images of **pristine material**

Critic **tested** with images of potentially **altered material** morphology -> Image scores

Generator
- 3 up-sampling/convolutional (ReLu)/batch normalization layers, 1 convolutional (Tanh) layer
- Filters 256-128-64-32

Critic
- 7 convolutional layers (LeakyReLu)
- Filters 32-32-64-64-128-128-256

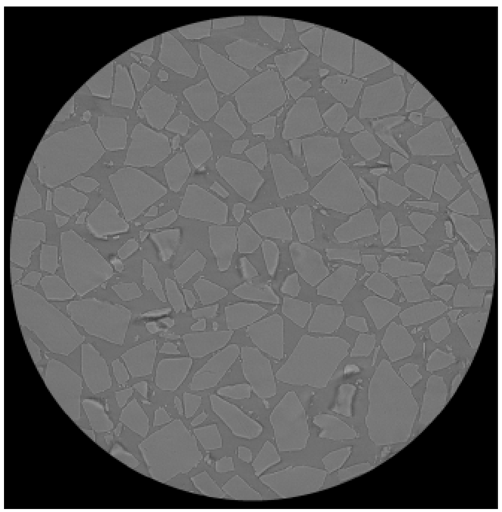
[1] Hsu, T., et al., *Microstructure Generation via Generative Adversarial Network for Heterogeneous, Topologically Complex 3D Materials.* Jom, 2020

Data

Training

CT scan of pristine Pharmatose

- 1800 2d images
- Each 2d image 2,000x2,000 pixels
- Batch: 64 down-sampled (1/4) 512x512 cropped segments

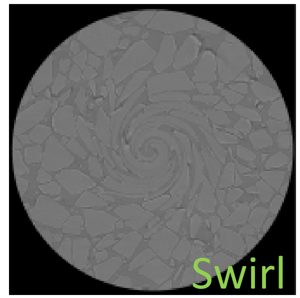


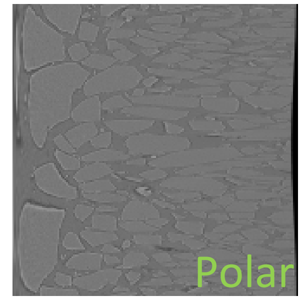
HMX microstructure generation with single 3,000x3,000 pixel SEM image [1]

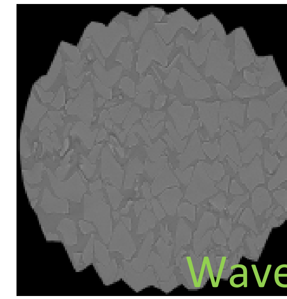
[1] Chun, S., et al., *Deep learning for synthetic microstructure generation in a materials-by-design framework for heterogeneous energetic materials.* Scientific Reports, 2020. **10**(1).

Testing

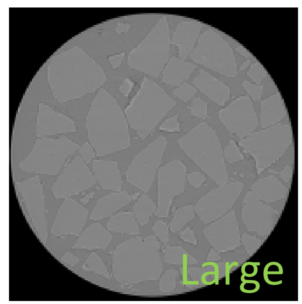
Image Transformations

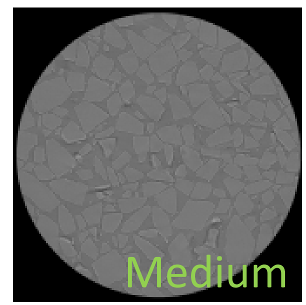


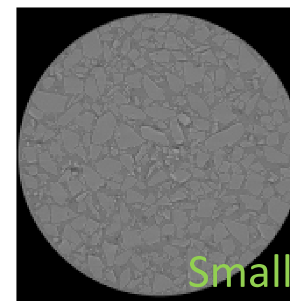




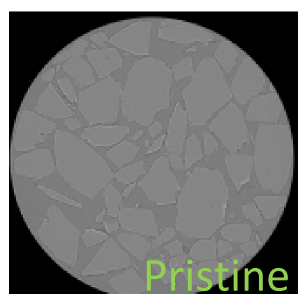
Varying Particle Sizes

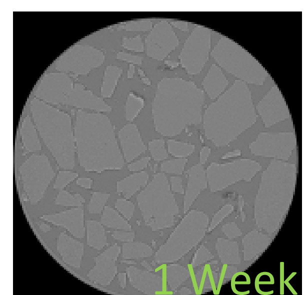


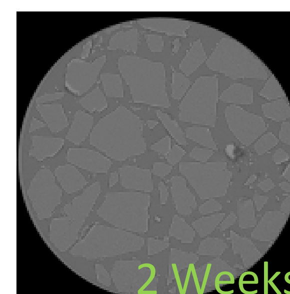




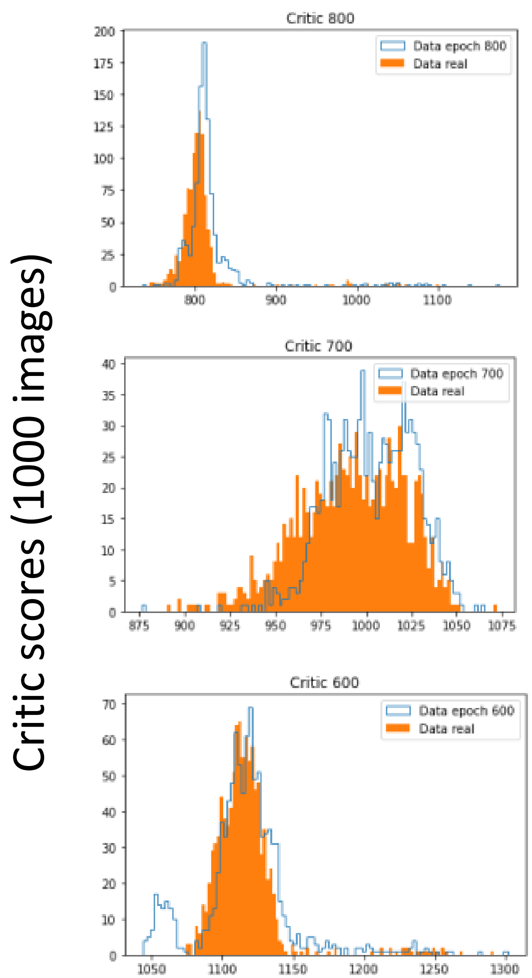
Aged Material (120°C)

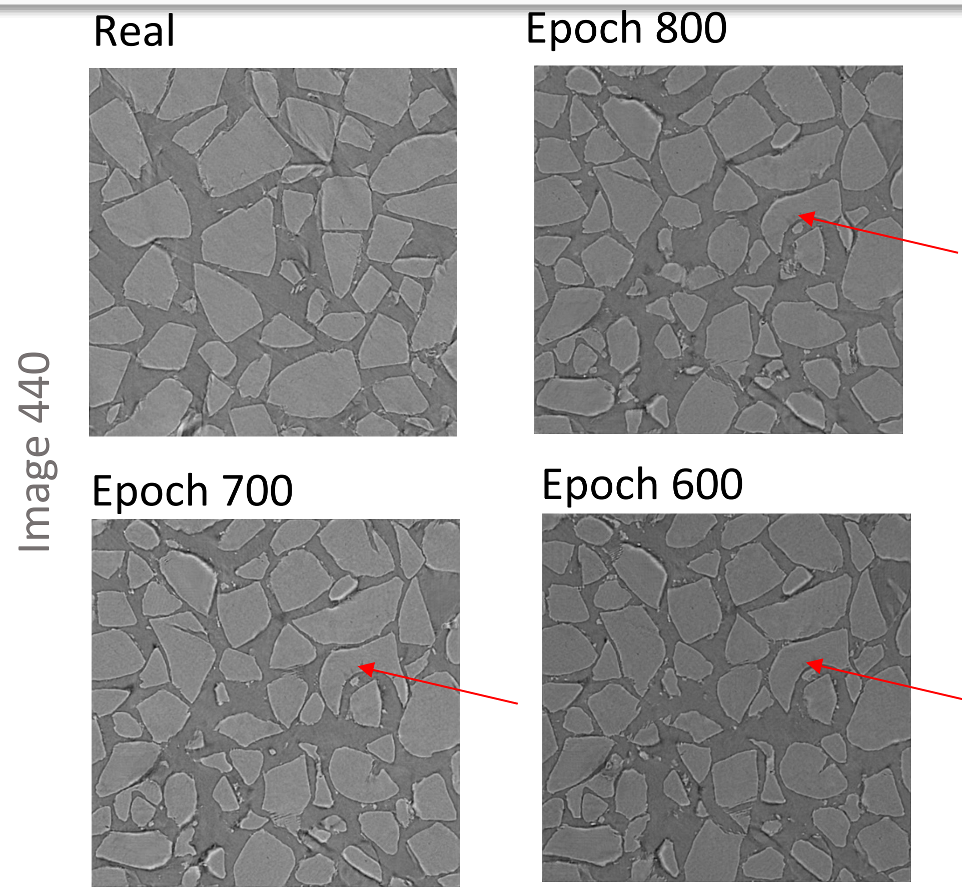






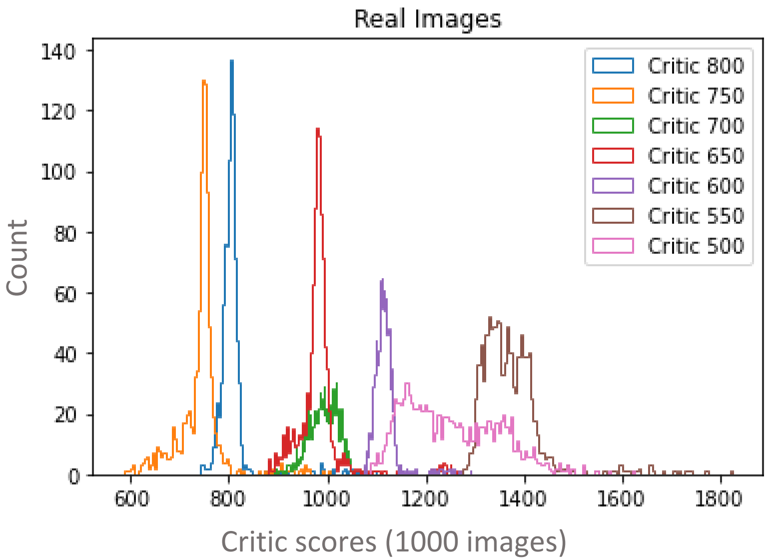
Results – Image Generation



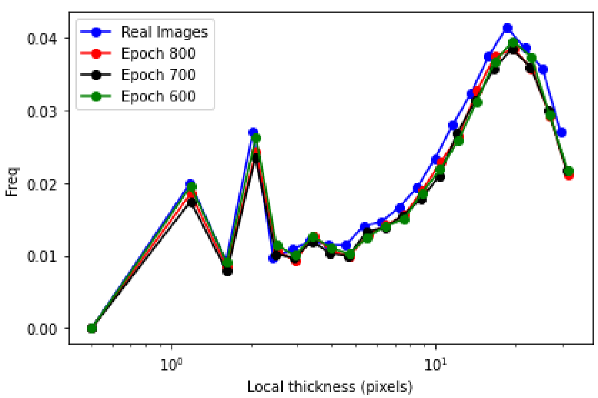


- For a given epoch, the critic scores real and fake images similarly
- Scores vary significantly between epochs
- “Blobs” in fake images don’t seem to improve
- Training restriction 512x512 pixels image size

Results – Image Generation

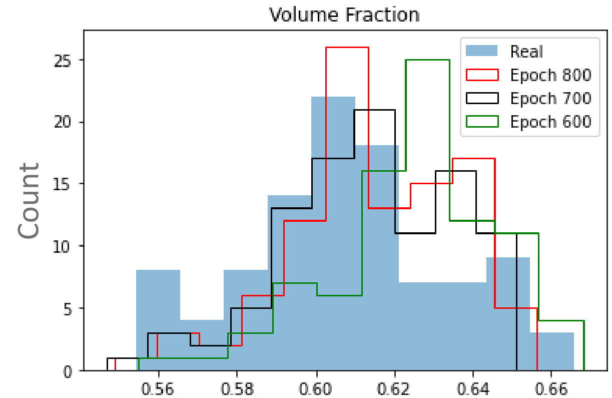


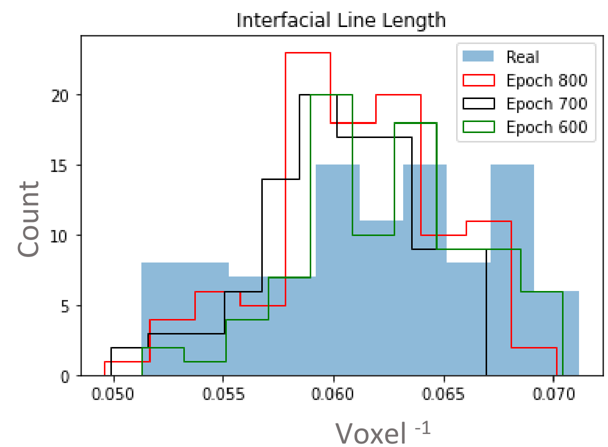
Converging?



Despite “blobs” image properties appear to be well reproduced

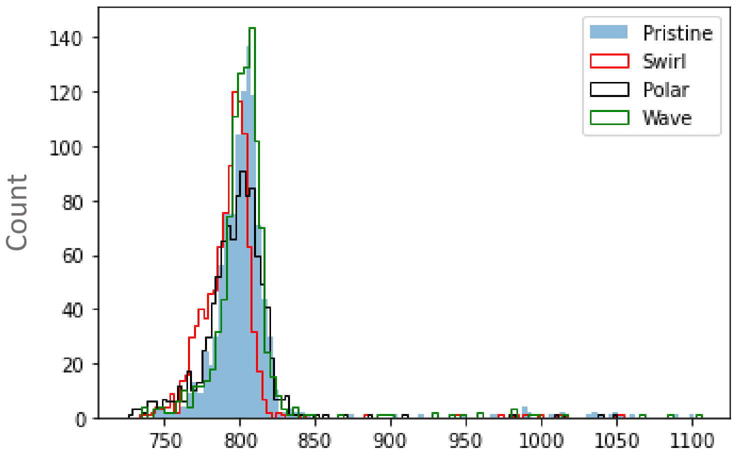
100 images



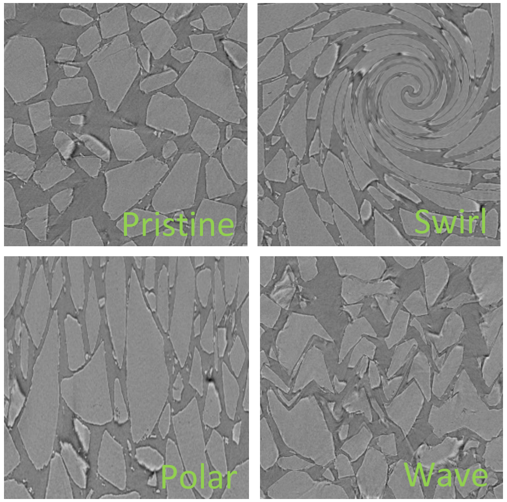


- Volume fraction: epoch 800 closest to real images
- Interfacial line length: different epochs similar distribution

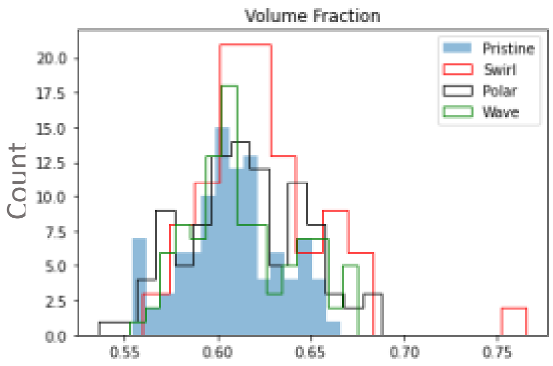
Results – Scores for transformed images

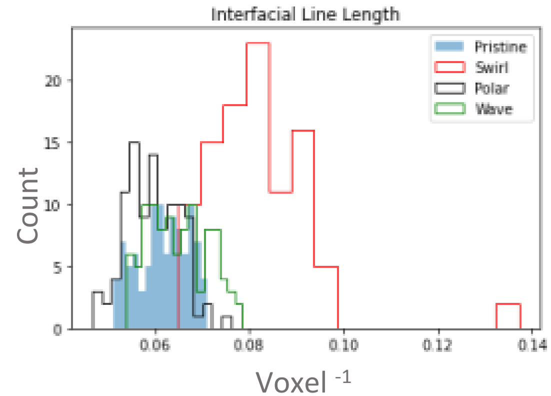


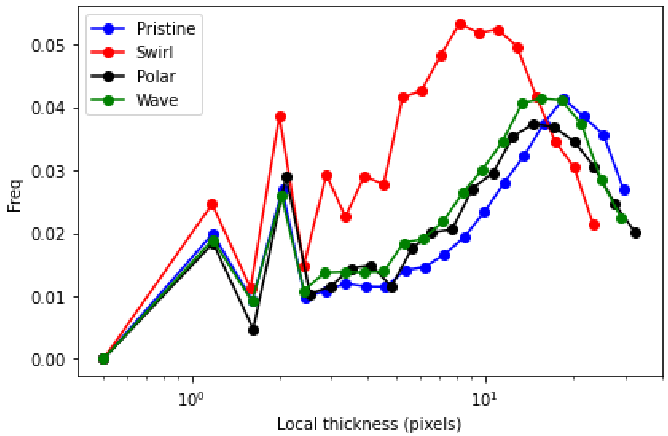
Critic scores (1000 images, critic epoch 800)



100 images

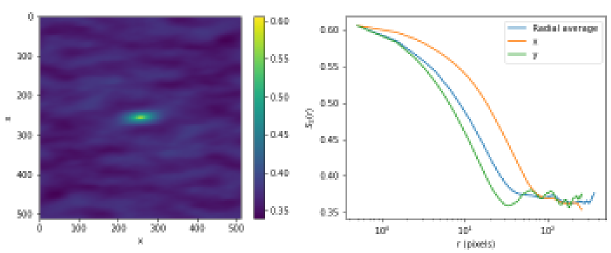






Although there is some response, critic is not sensitive enough to pick up differences in particle shape

Two-point correlation function
Example image, polar transformation



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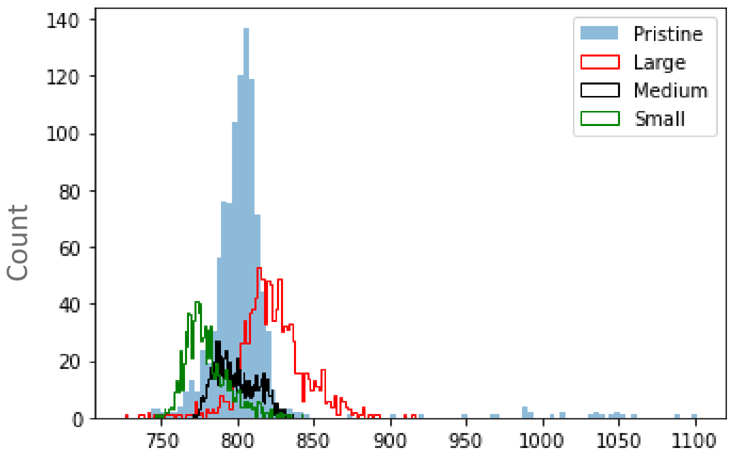
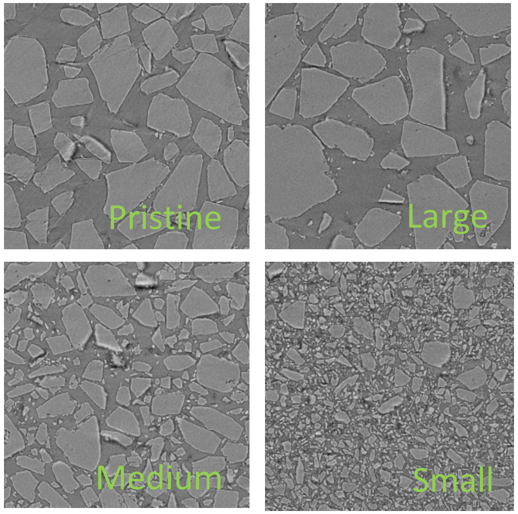
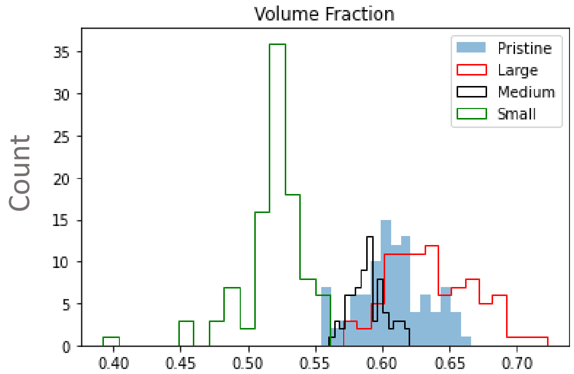
Results – Scores for varying particle sizes

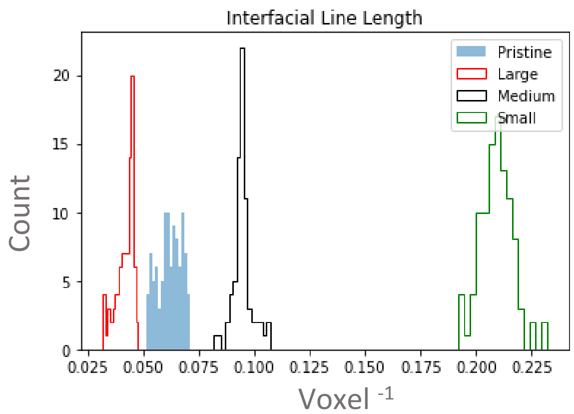


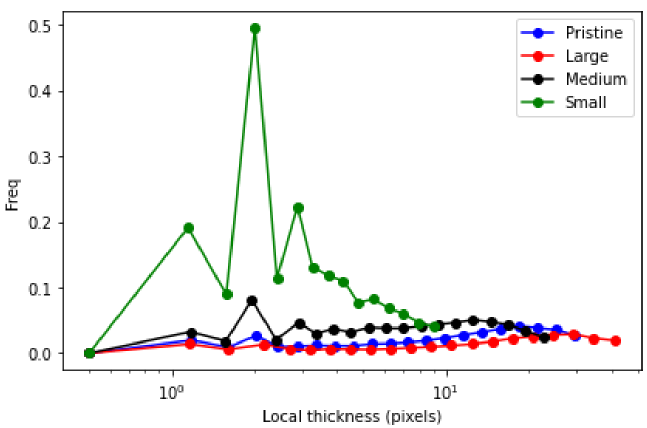
Critic scores (1000 images, critic epoch 800)



100 images





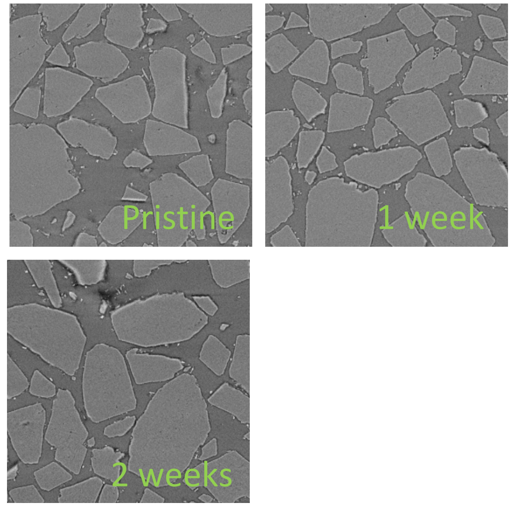


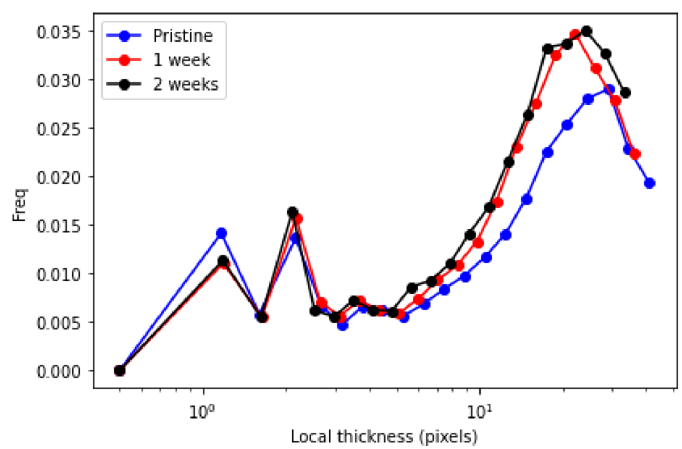
Critic scores images of different particle sizes differently and in consistent order

Results – Scores for aged data

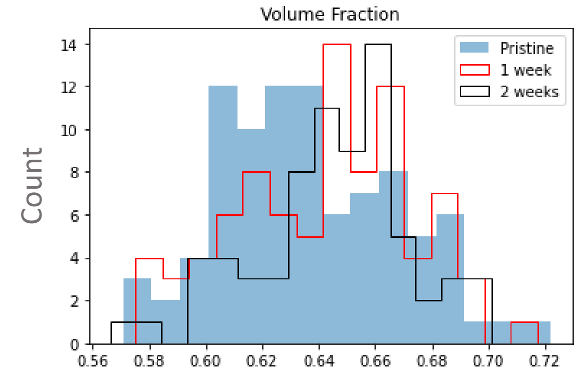
- Network training in progress
- Scores will be available soon

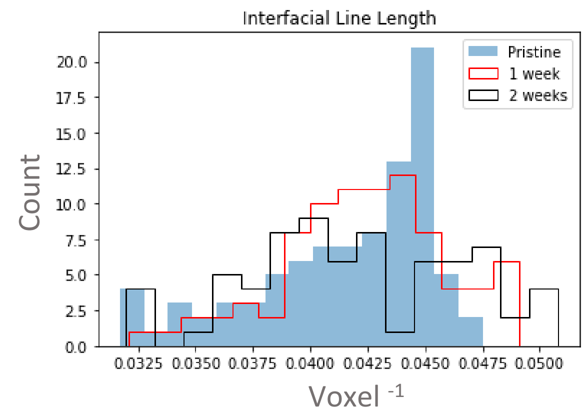
Unlikely, that critic scores can differentiate between materials …





100 images





Only subtle differences between pristine and aged material using traditional metrics.

Conclusions

Concept works, the critic of a GAN can be used as a detector of morphological change but significant improvements needed before the critic can be used in practice:

- Image generation without “blobs”
- Increase critic sensitivity
- Increase of training image size

Help (ideas, collaborations) from ML/DL community very much appreciated

Potentially interested customers: NA-193, Aging & Lifetimes