

# Microstructure Quantification With Deep Learning Encoders Pre-Trained on a Massive Microscopy Dataset

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Joshua Stuckner  
Nasa Glenn Research Center  
Materials Informatics Scientist

## Collaborators

Dr. Joshua Stuckner, Dr. Bryan Harder, Dr. Timothy M. Smith,  
Dr. Steven M. Arnold, Thomas Ciardi

## Funding

Congress

↳ NASA

↳ Aeronautics Research Mission Directorate (ARMD)

↳ Transformative Aeronautics Concept Program (TACP)

↳ Transformational Tools and Technology (T<sup>3</sup>)

National  
aeronautics and  
Space  
Administration

Processing  $\rightarrow$  Properties

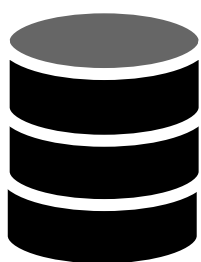
Properties  $\rightarrow$  Processing

$x$

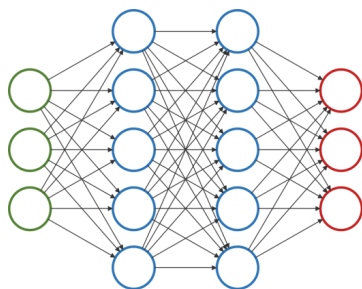
$y$

$$y = F(x)$$

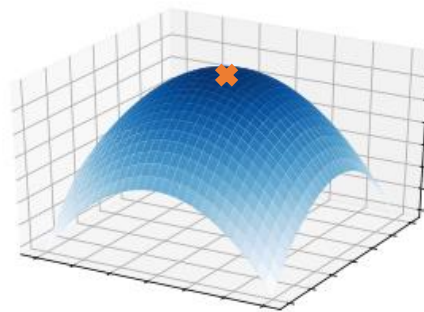
processing:  $x^* = \operatorname{argmax}(F(x))$



Data



ML Model

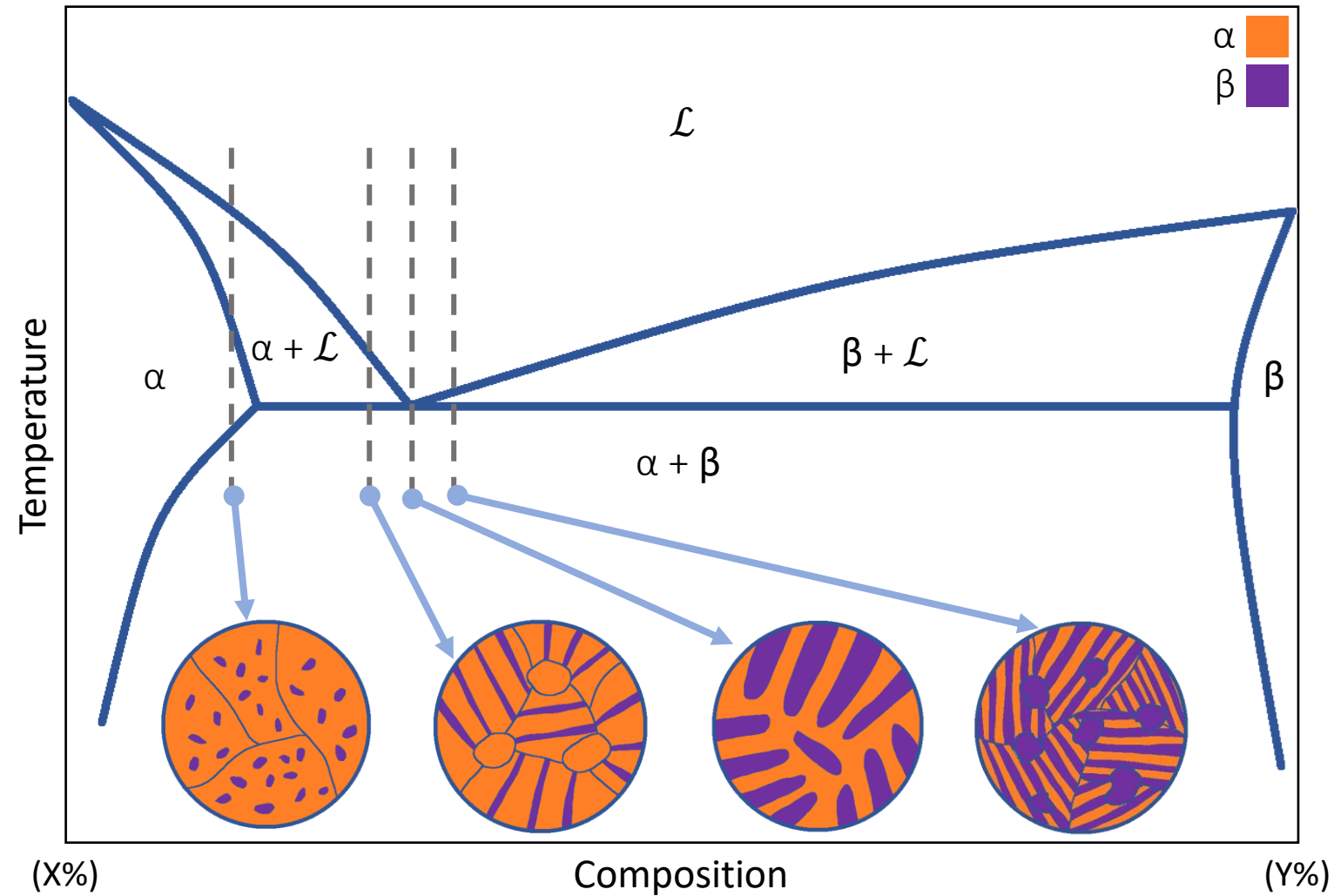


Optimizer



Processing

## Phase Diagram



Processing  $\rightarrow$  Structure  $\rightarrow$  Properties  
x z y

$$y = F(x, z)$$

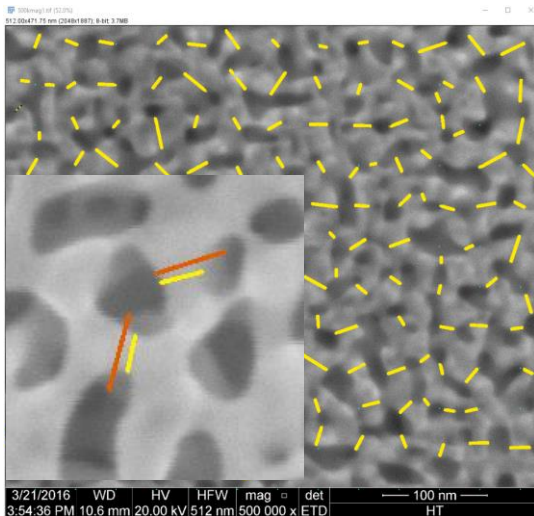
Problem: How do we quantify the structure

## 1. Manual Quantification

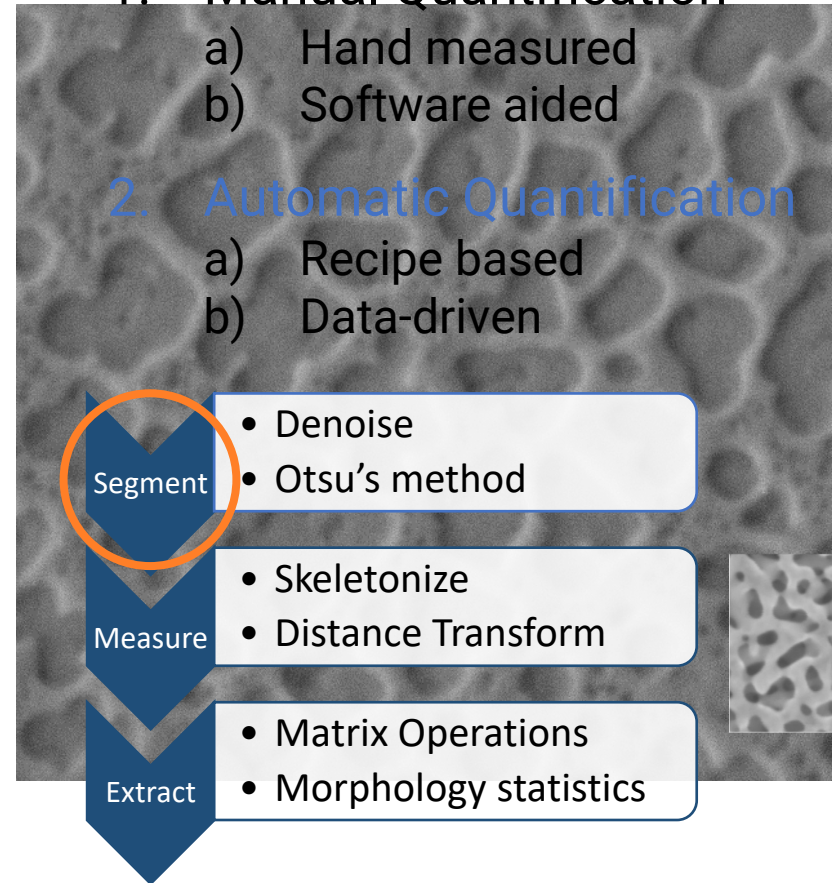
- a) Hand measured
- b) Software aided

## 2. Automatic Quantification

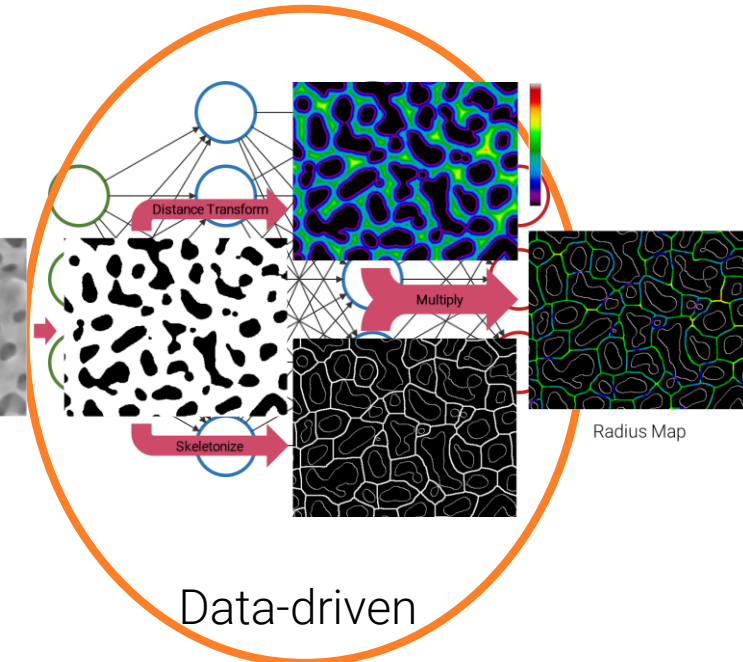
- a) Recipe based
- b) Data-driven



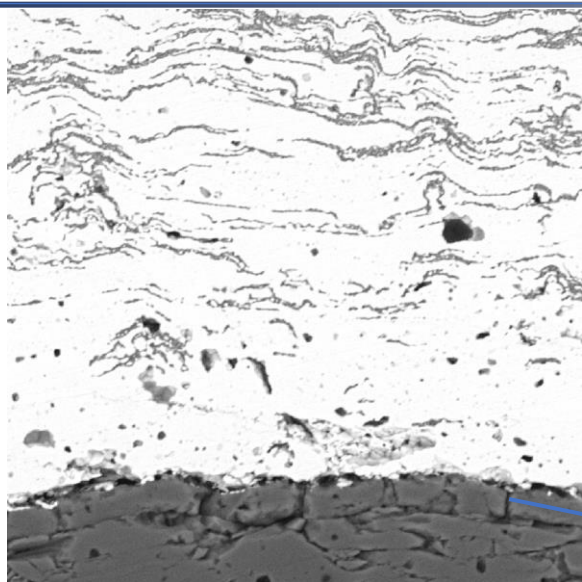
Manual



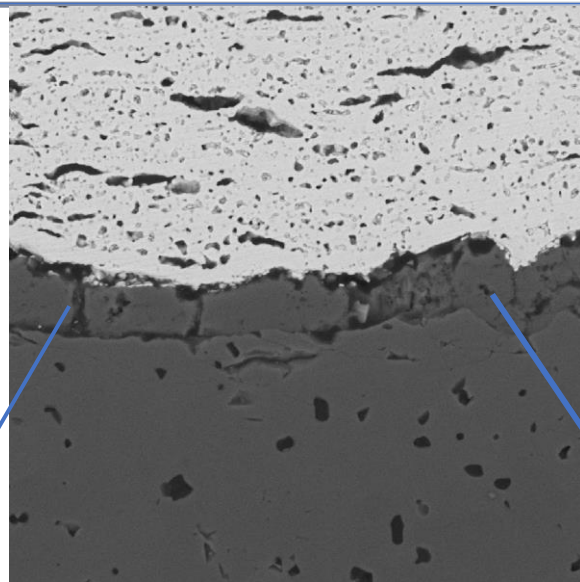
Recipe based



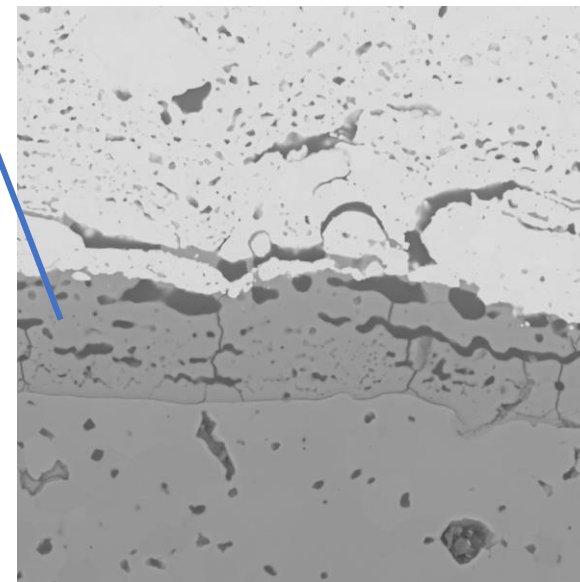
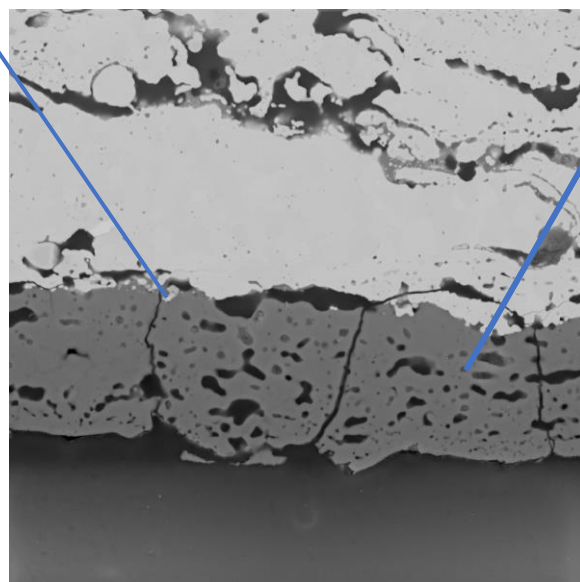
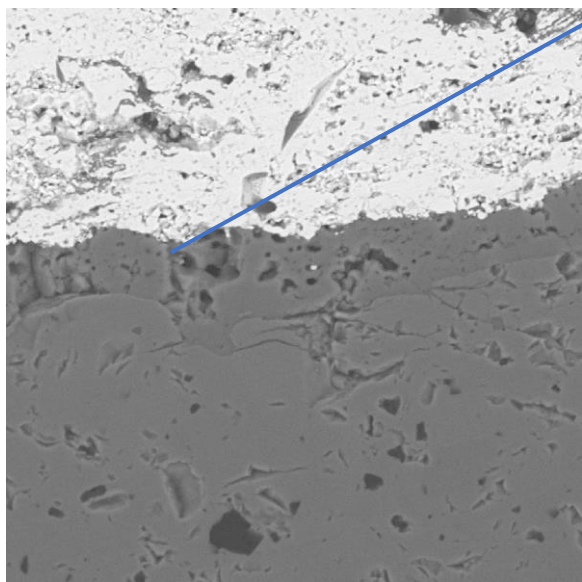
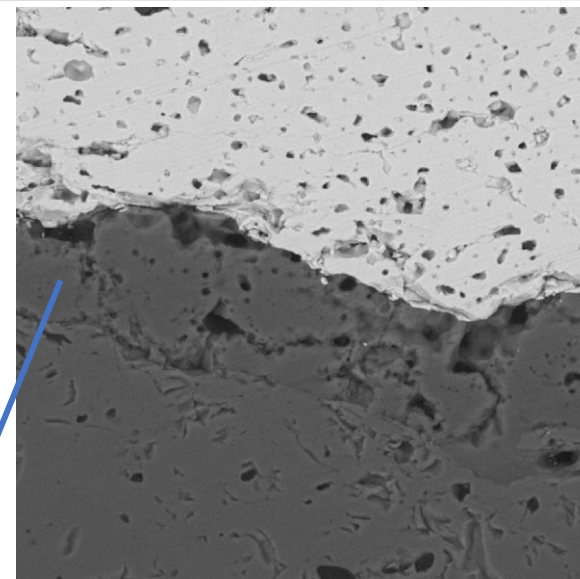
Data-driven

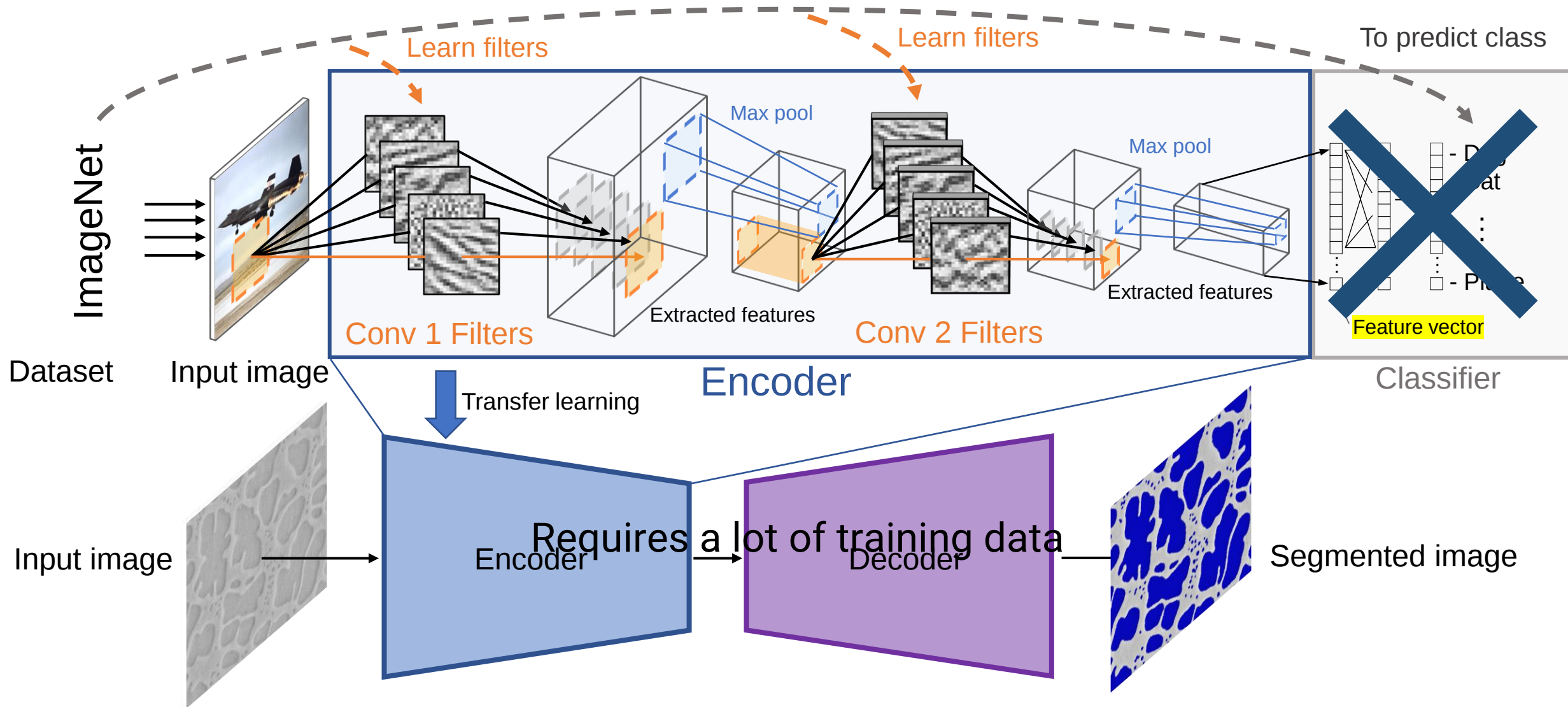


Crack

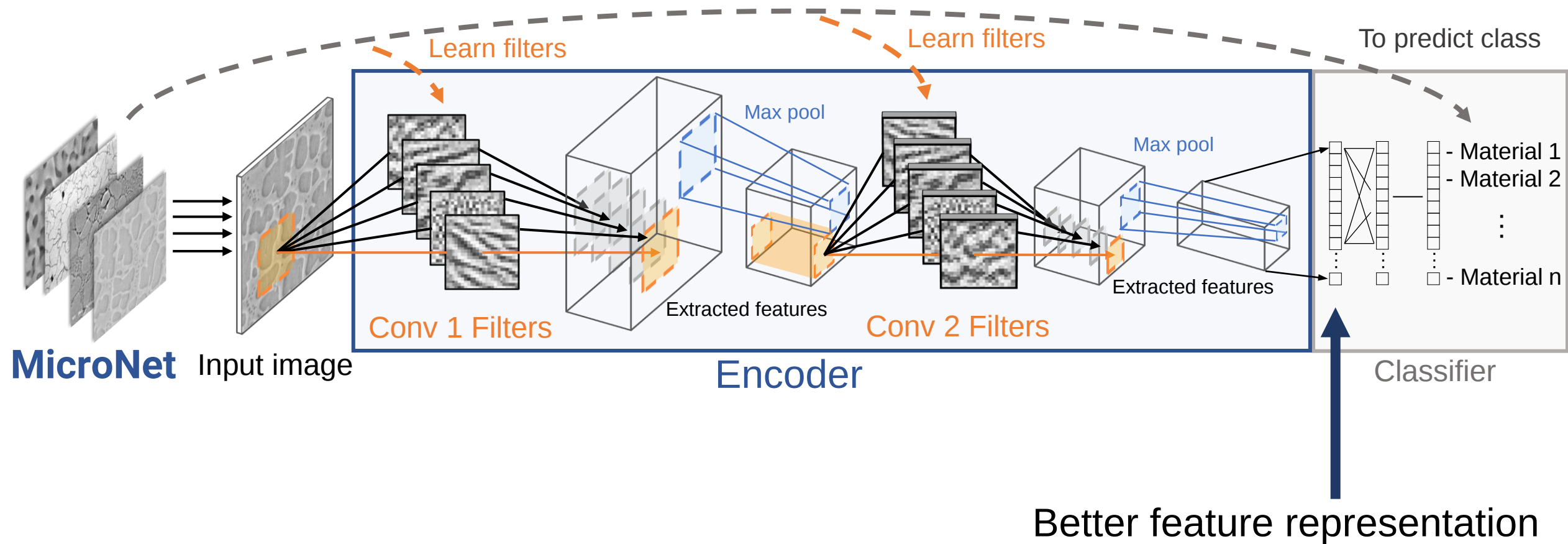


Oxide  
Layer

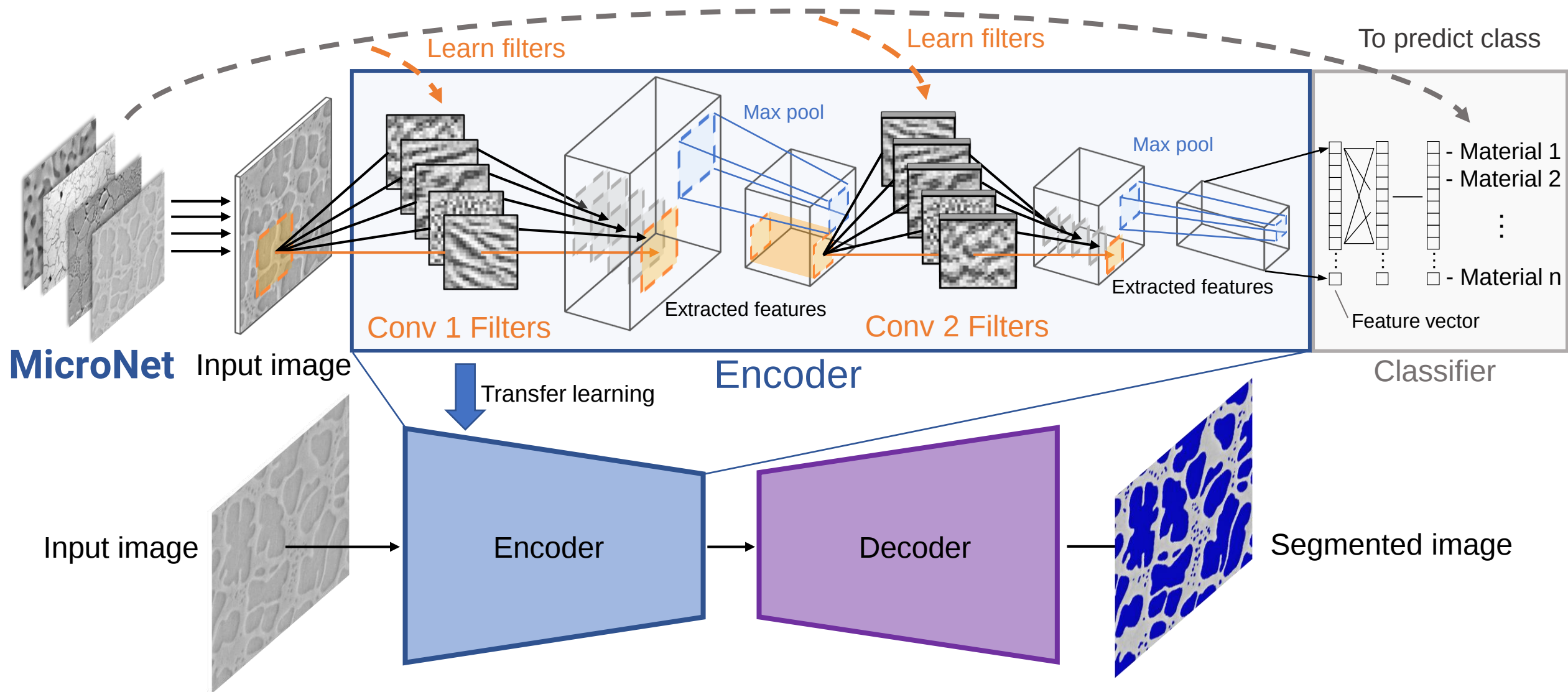




# CNNs



# CNNs



# Classification Training

## Data

- Classes: 54
- Size: 1057 x 750, 150 GB
- Training set: 108,161
- Validation set: 2700 (50/class)

## Augmentation

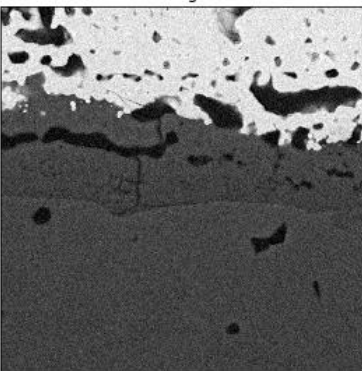
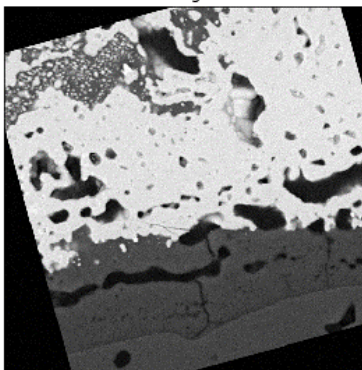
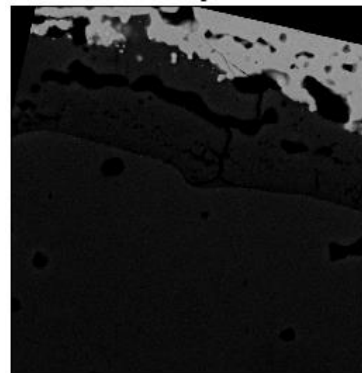
- Random crop, resize, flip, mirror, rotate
- Contrast, CLAHE, Brightness, Gamma, Hue/Saturation
- Gaussian Noise
- Sharpen
- Blur

## Training

- Early stopping
- Learning rate decay

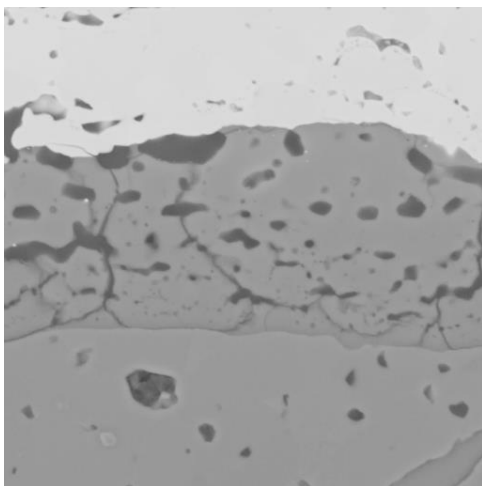
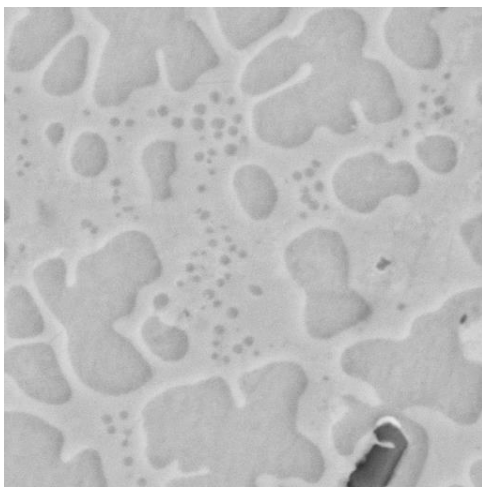
## Hardware

- 4 Nvidia Quadro V100 32 GB



## Encoders

- |                     |                       |
|---------------------|-----------------------|
| • resnet18          | • senet154            |
| • resnet34          | • se_resnet50         |
| • resnet50          | • se_resnet101        |
| • resnet101         | • se_resnet152        |
| • resnet152         | • se_resnext50_32x4d  |
| • resnext50_32x4d   | • se_resnext101_32x4d |
| • resnext101_32x4d  | • densenet121         |
| • resnext101_32x8d  | • densenet169         |
| • resnext101_32x16d | • densenet201         |
| • resnext101_32x32d | • densenet161         |
| • resnext101_32x48d | • inceptionresnetv2   |
| • dpn68             | • inceptionv4         |
| • dpn68b            | • efficientnet-b0     |
| • dpn92             | • efficientnet-b1     |
| • dpn98             | • efficientnet-b2     |
| • dpn107            | • efficientnet-b3     |
| • dpn131            | • efficientnet-b4     |
| • vgg11             | • efficientnet-b5     |
| • vgg11_bn          | • efficientnet-b6     |
| • vgg13             | • efficientnet-b7     |
| • vgg13_bn          | • mobilenet_v2        |
| • vgg16             | • xception            |
| • vgg16_bn          |                       |
| • vgg19             |                       |
| • vgg19_bn          |                       |

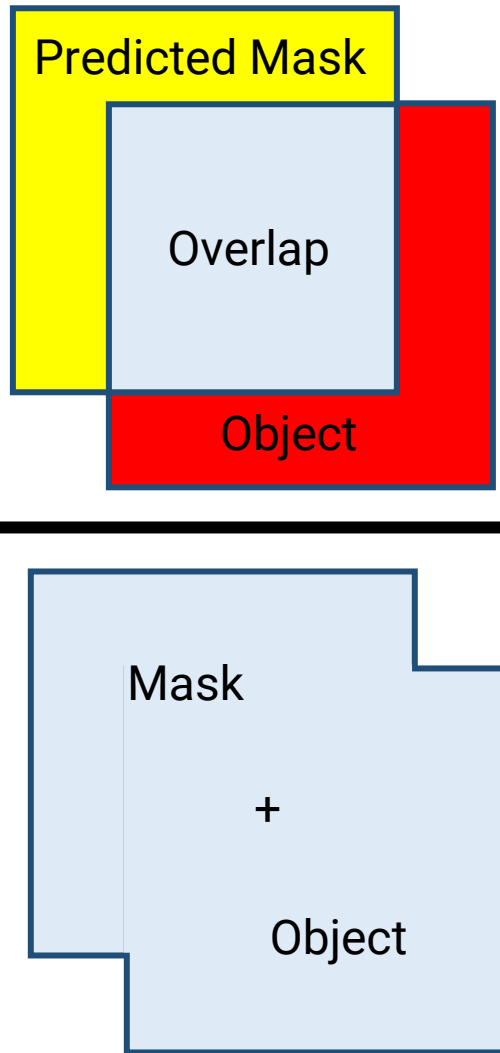


| Experiment | # Train | # Val | # Test |
|------------|---------|-------|--------|
| Super-1    | 10      | 4     | 4      |
| Super-2    | 4       | 4     | 4      |
| Super-3    | 1       | 4     | 4      |
| Super-4    | 4       | 4     | 5*     |
| EBC-1      | 18      | 3     | 3      |
| EBC-2      | 4       | 3     | 3      |
| EBC-3      | 1       | 3     | 3      |

## Decoders

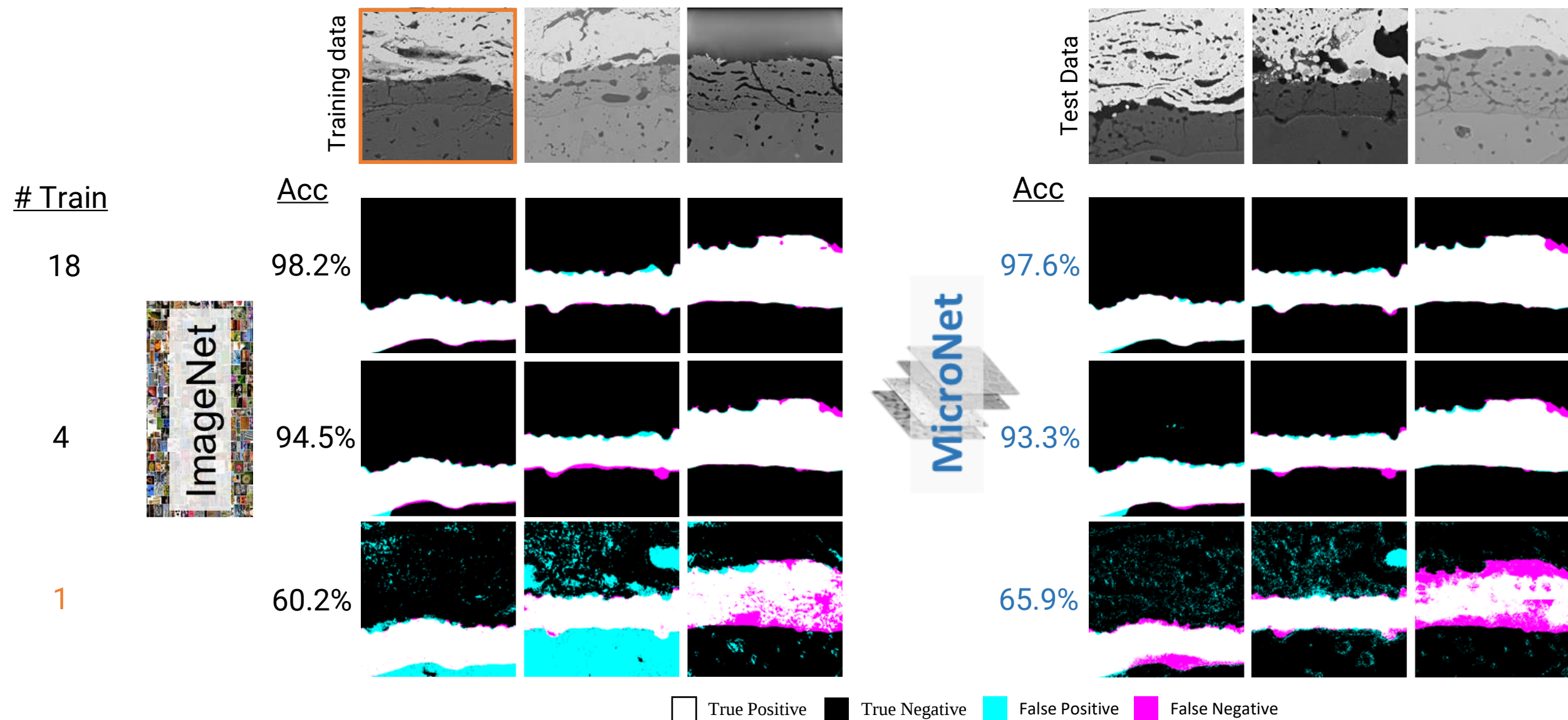
- UNet
- Unet++
- PSPNet
- FPN
- LinkNet
- PAN
- DeepLabV3+

**Accuracy:** Intersection over union (IoU)

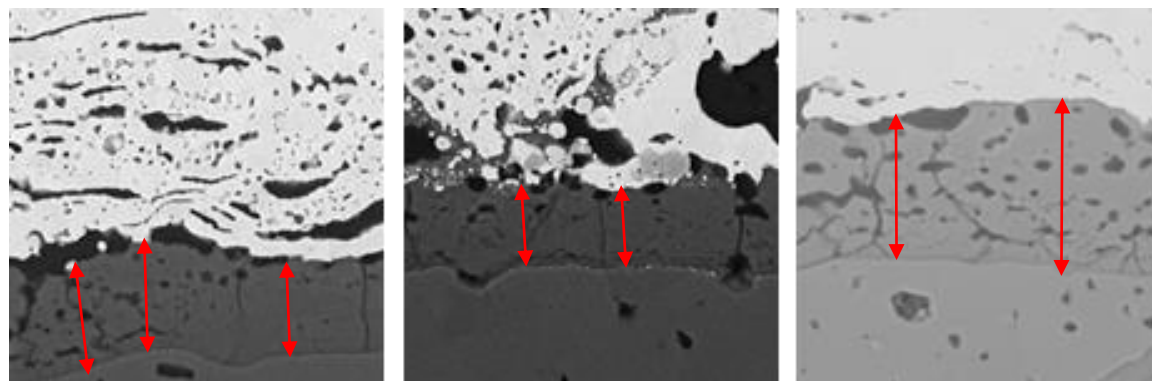
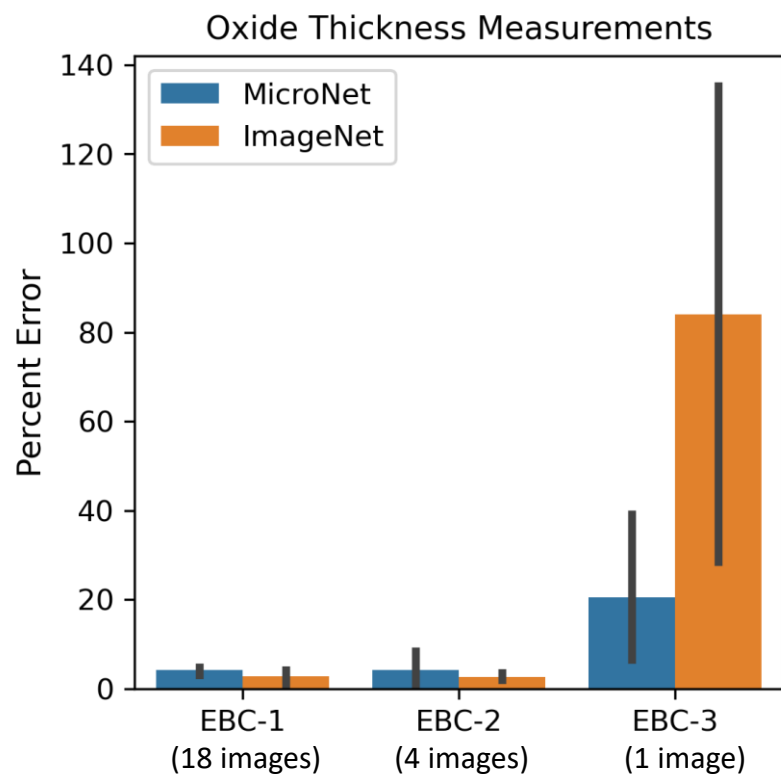
$$\text{IoU} = \frac{\text{Area of Overlap}}{\text{Area of Union}}$$


The diagram illustrates the components of the IoU formula. The top part shows a yellow rectangle labeled 'Predicted Mask' and a red rectangle labeled 'Object'. The intersection of these two rectangles is a light blue rectangle labeled 'Overlap'. The bottom part shows the union of the 'Mask' and 'Object' as a single light blue shape, labeled 'Mask + Object'.

# Segmentation

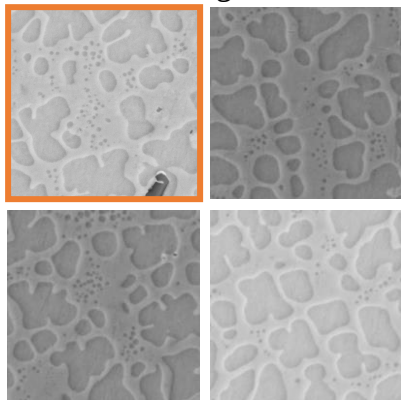


# Segmentation



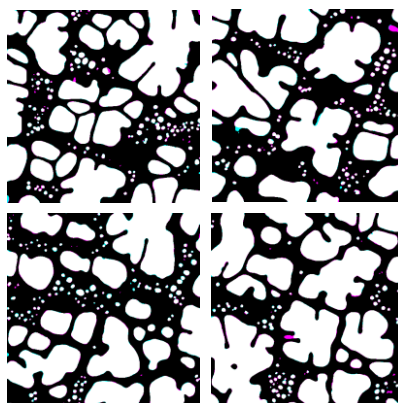
# Segmentation

Training data



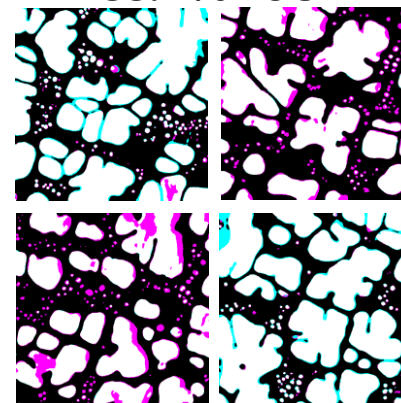
10 Images

96.5% IoU



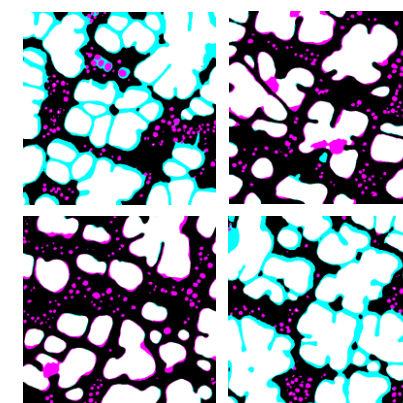
4 Images

88.7% IoU

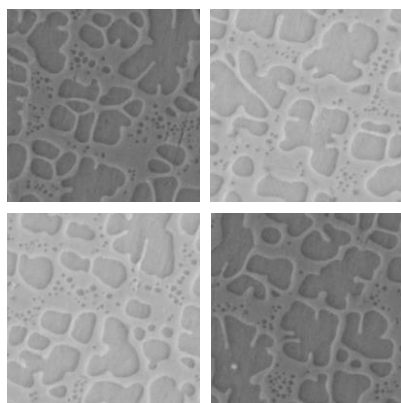


1 Images

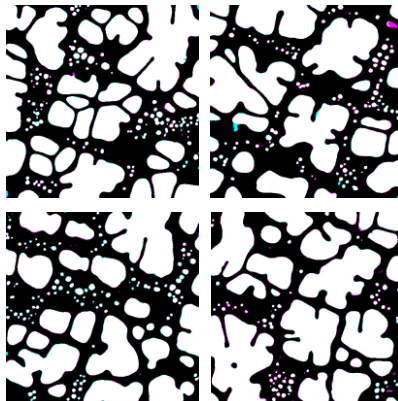
74.8% IoU



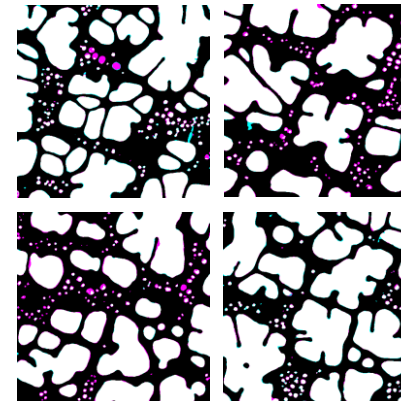
Test Data



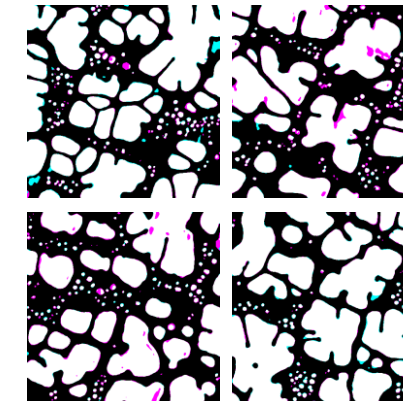
96.4% IoU



94.2% IoU



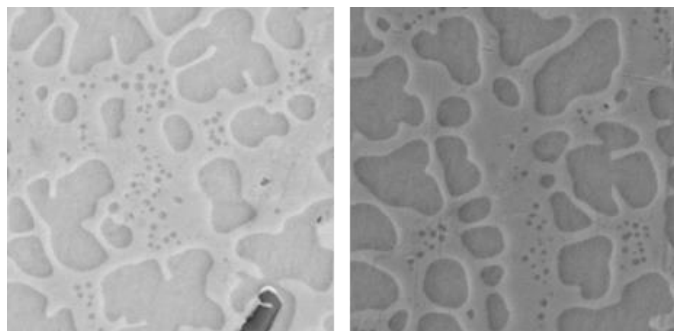
93.0% IoU



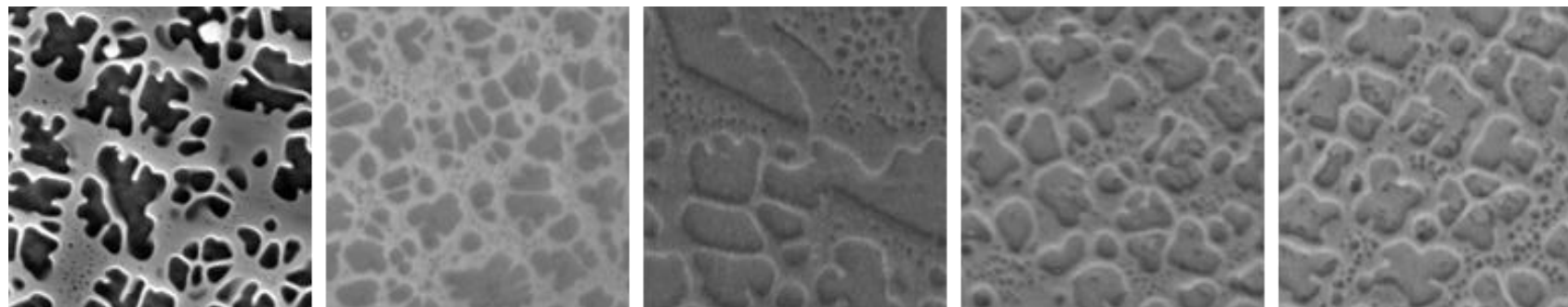
True Positive
  True Negative
  False Positive
  False Negative

# Segmentation

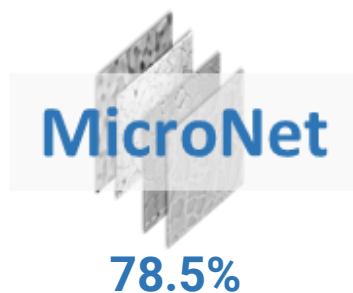
Training data



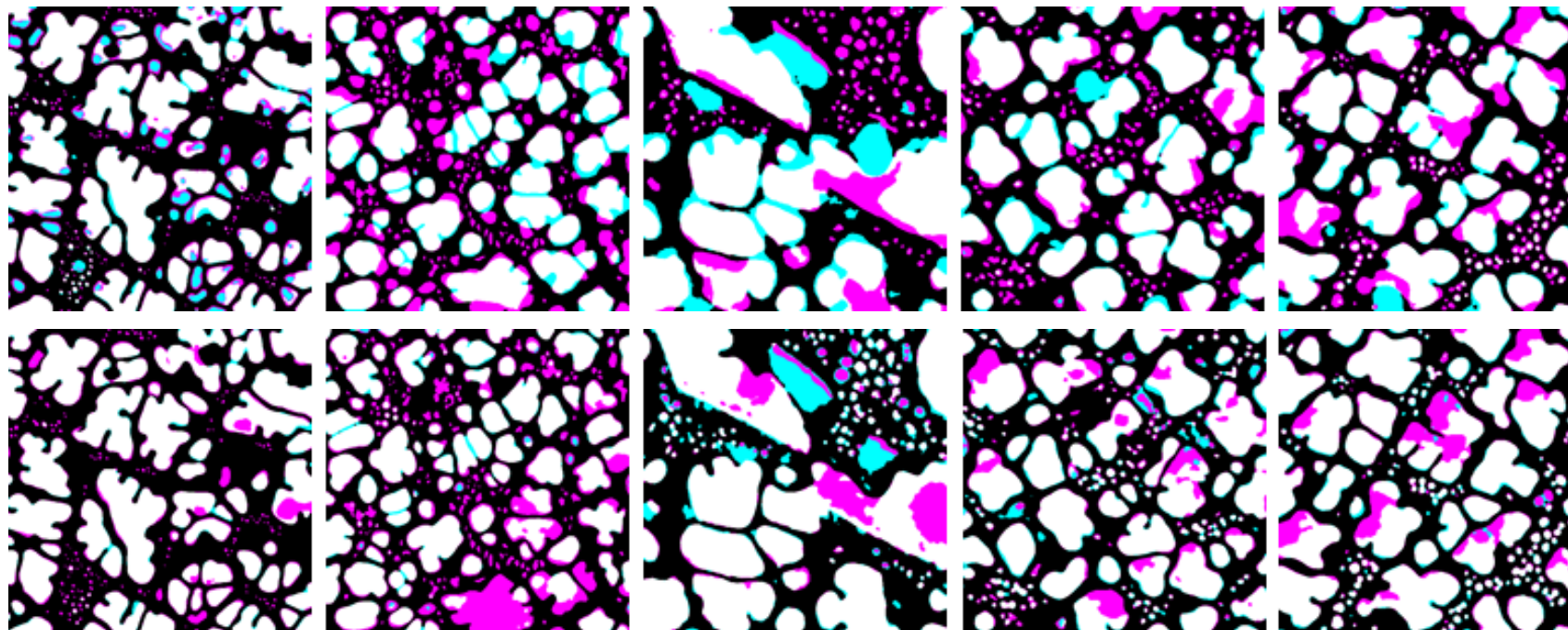
Test data



72.5%



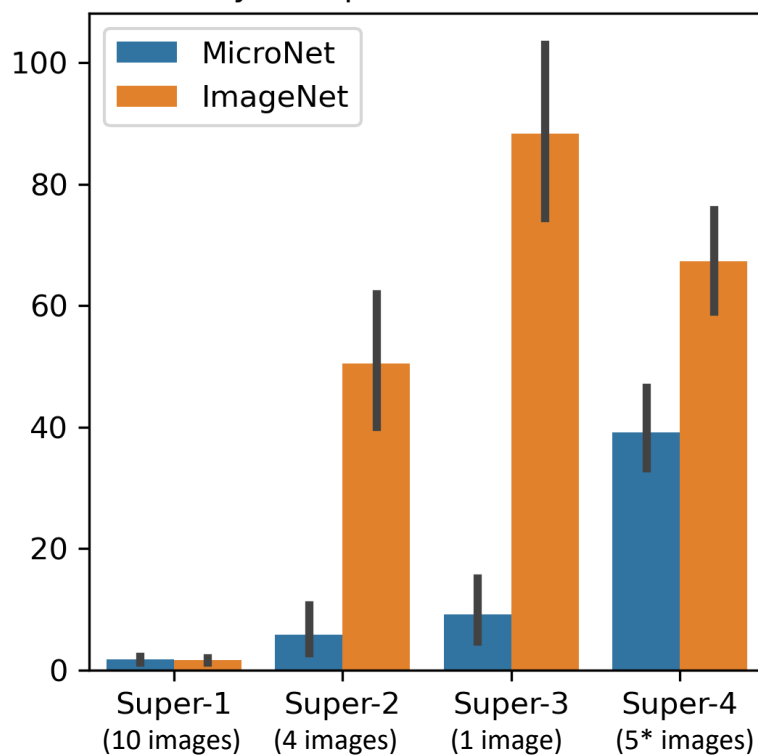
78.5%



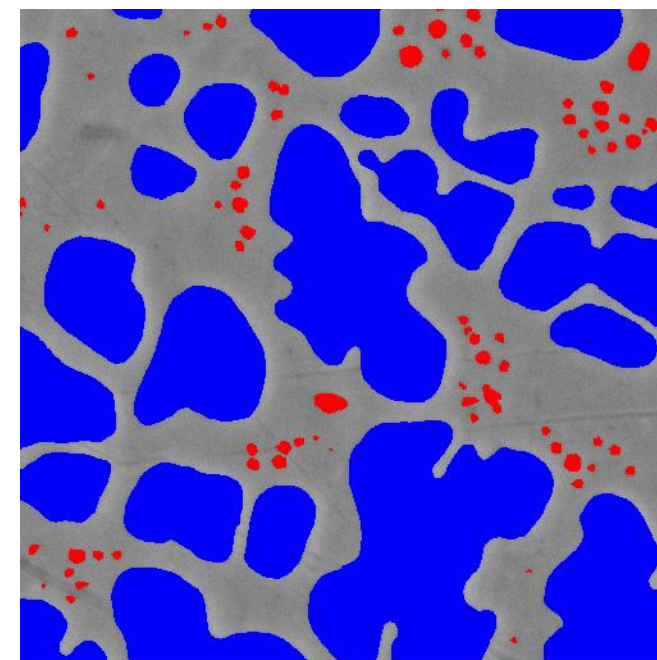
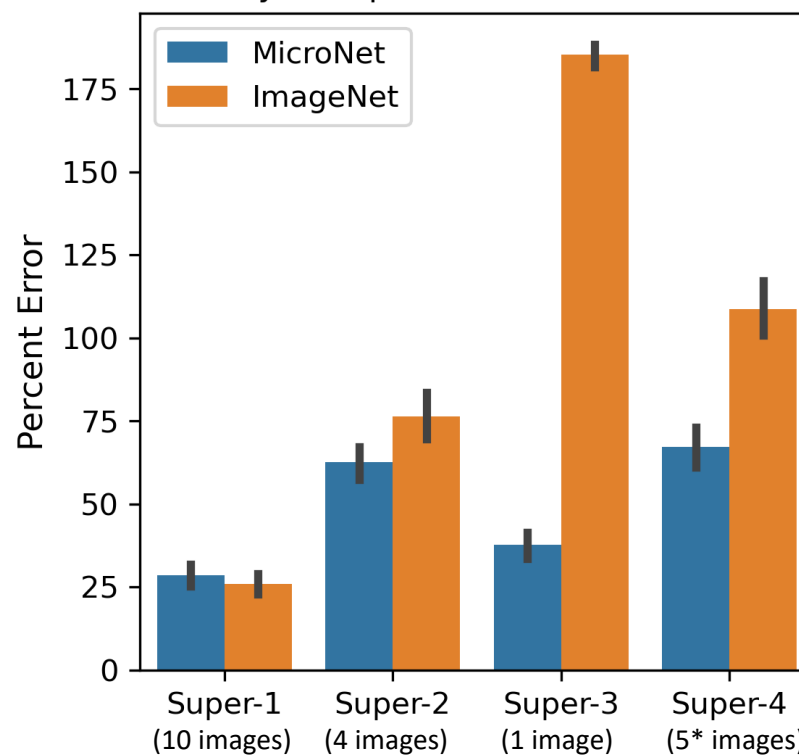
True Positive
  True Negative
  False Positive
  False Negative

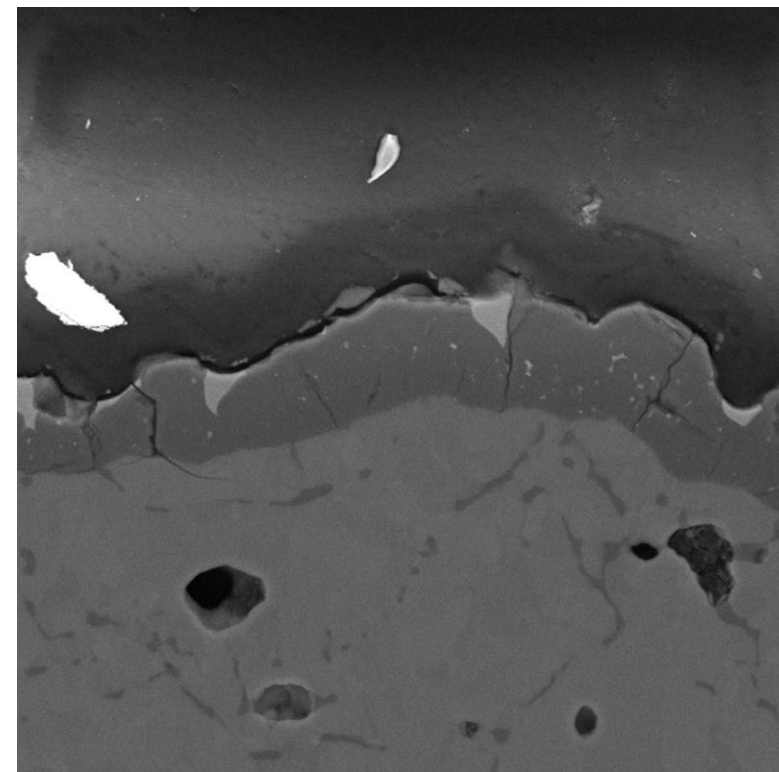
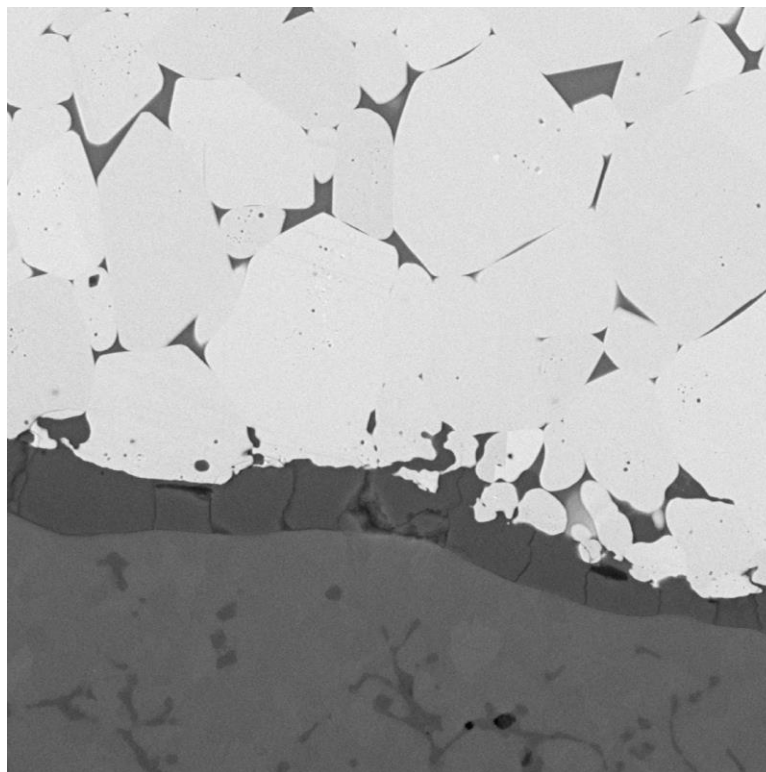
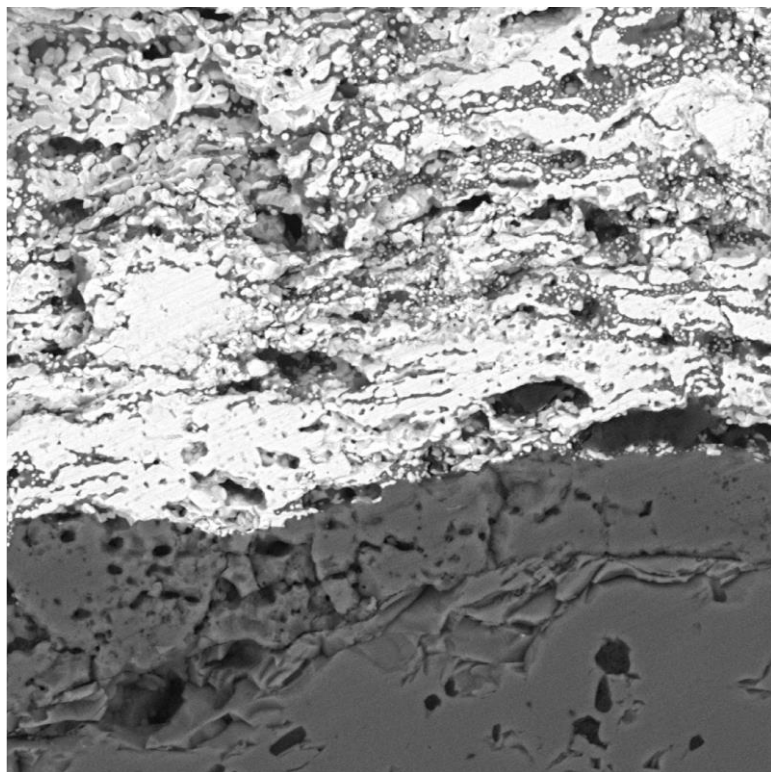
# Segmentation

Secondary Precipitate Size Measurements

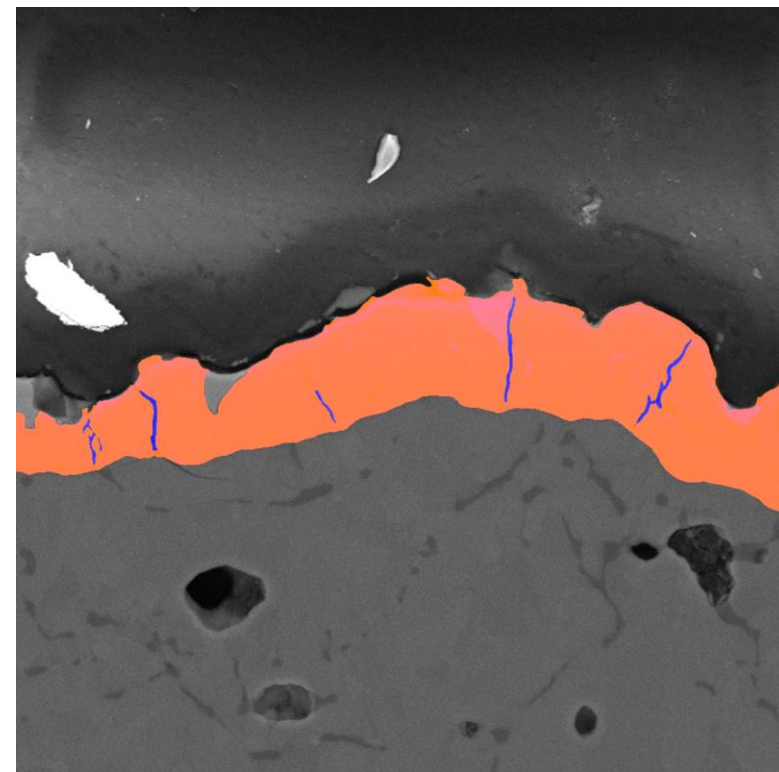
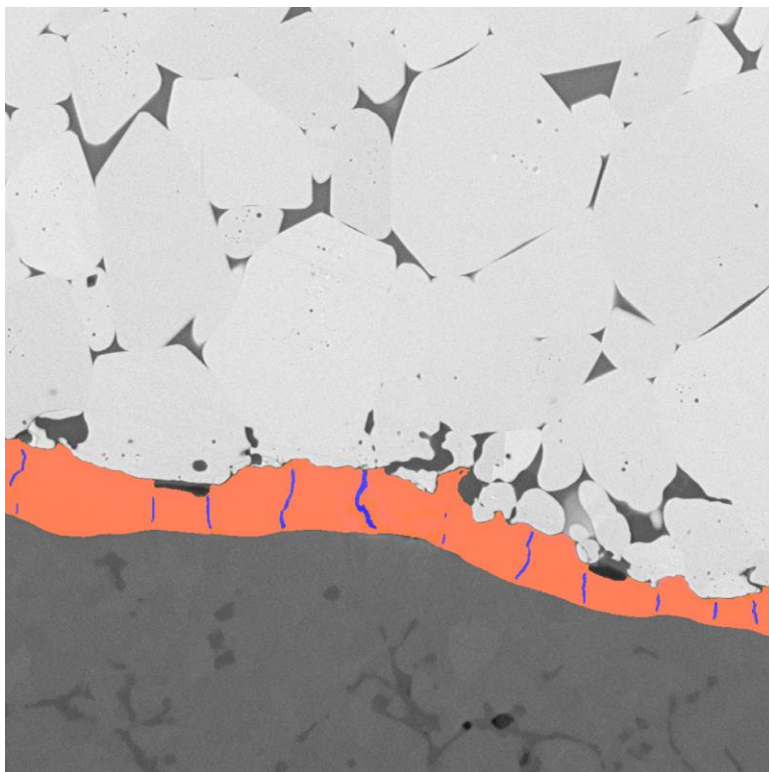
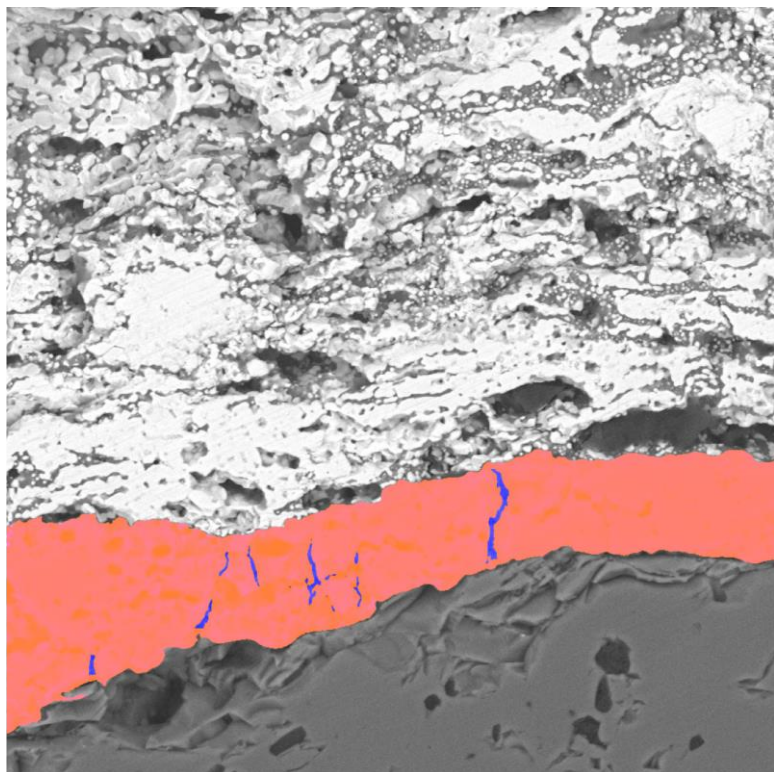


Tertiary Precipitate Size Measurements

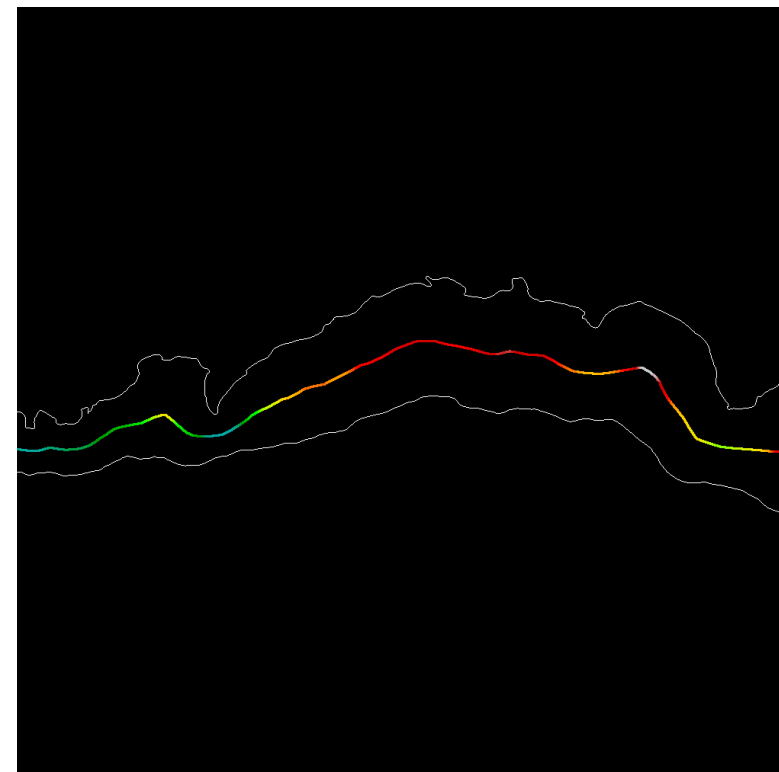
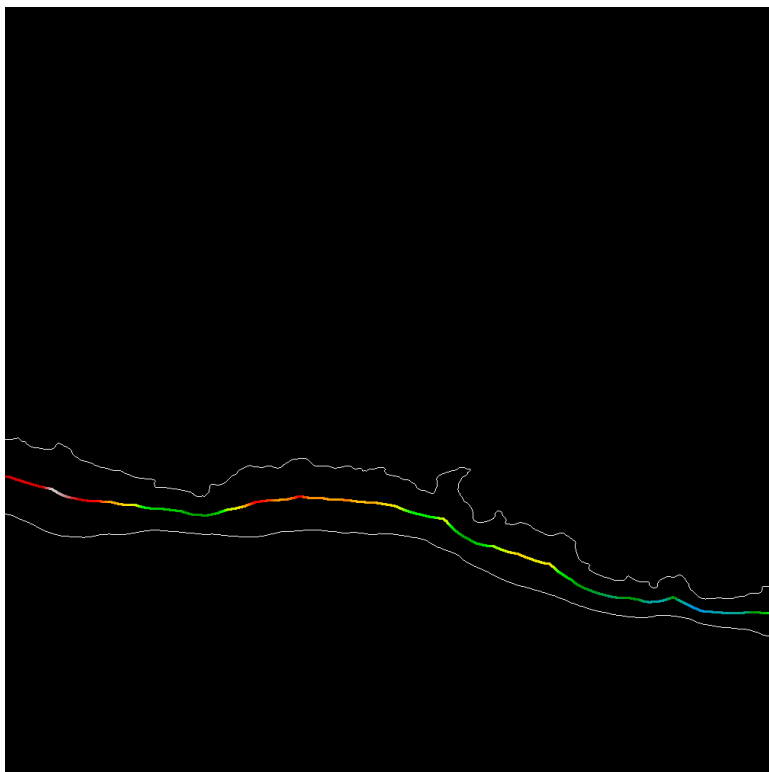
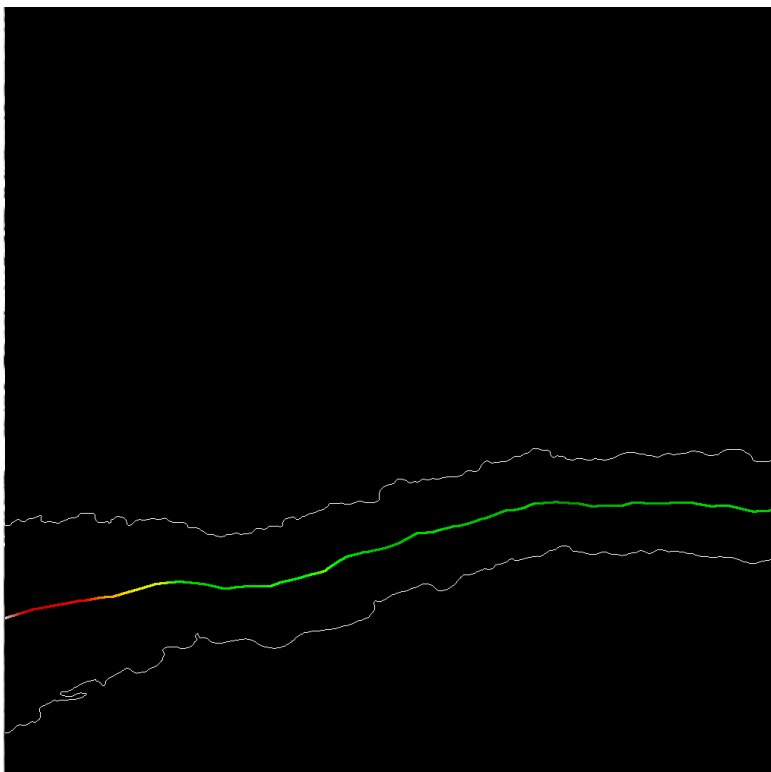




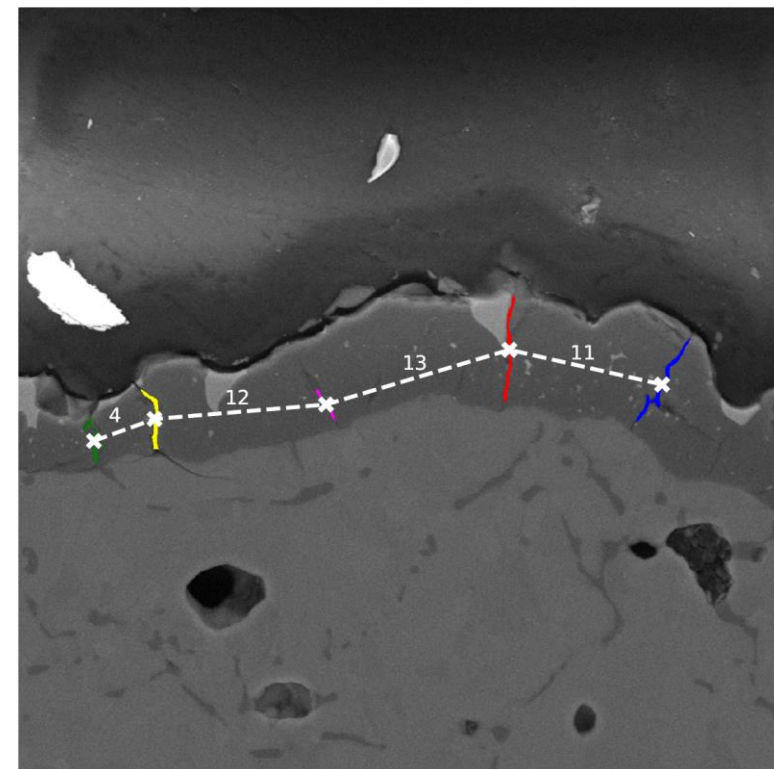
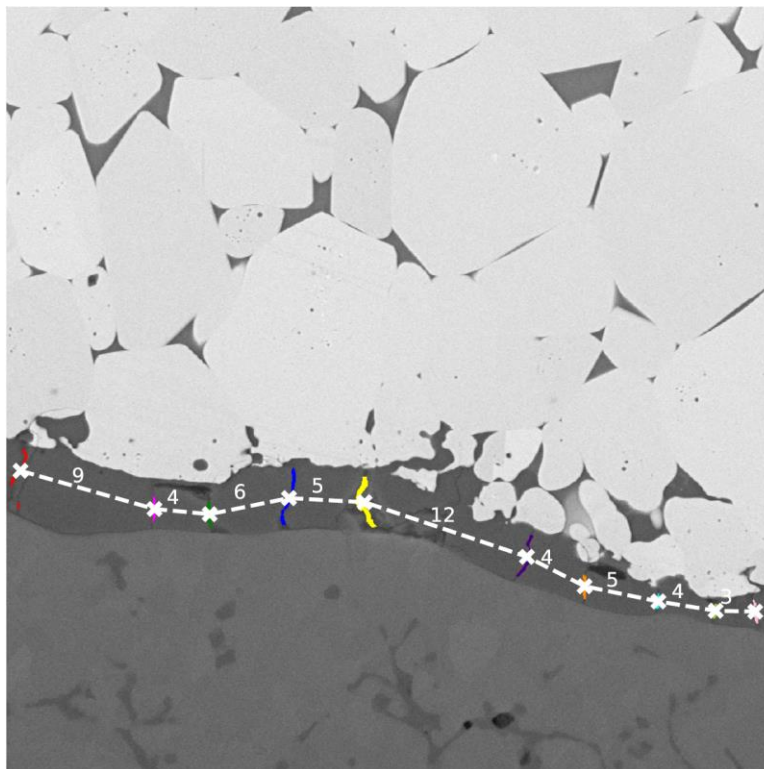
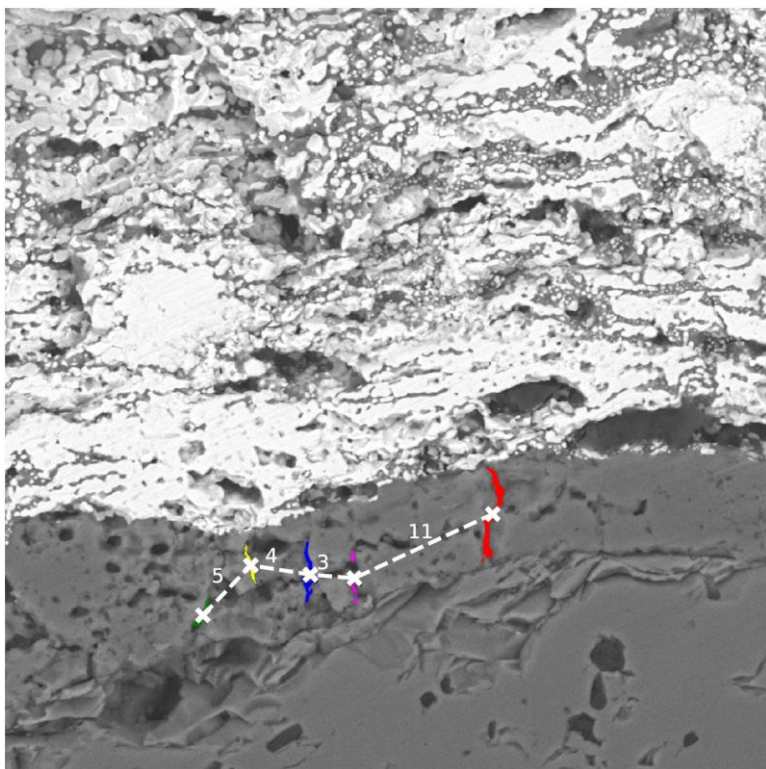
# Applications



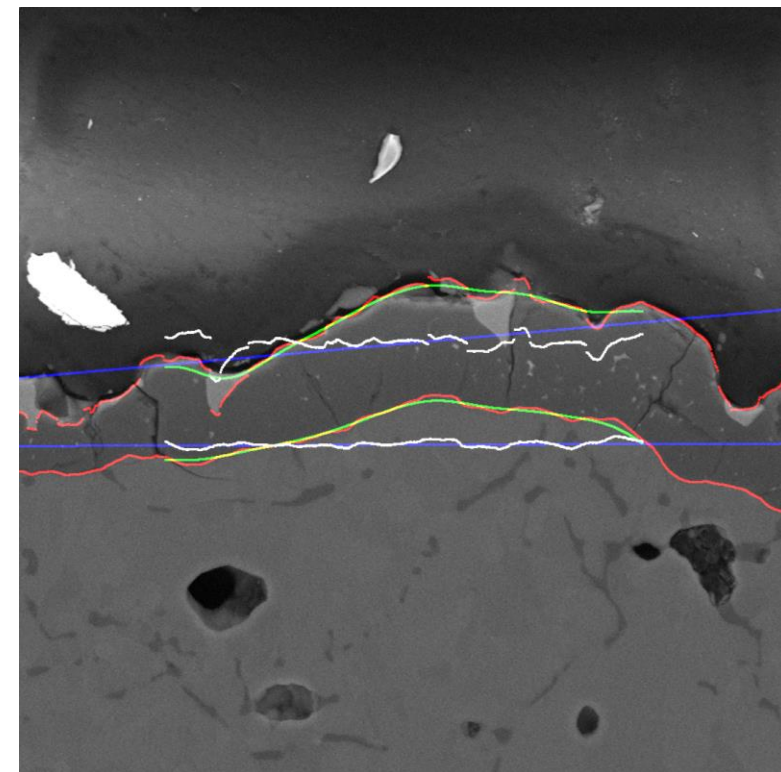
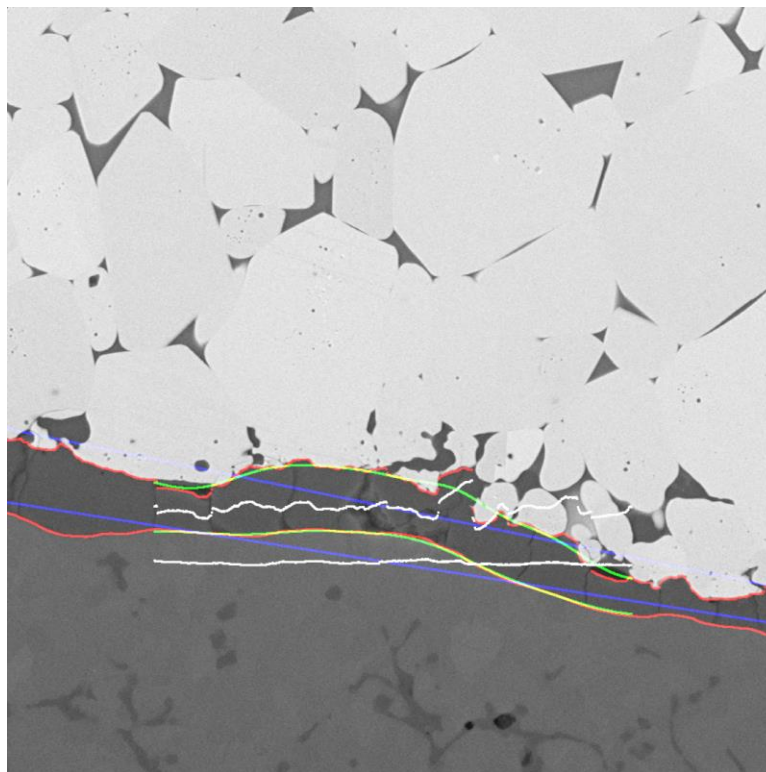
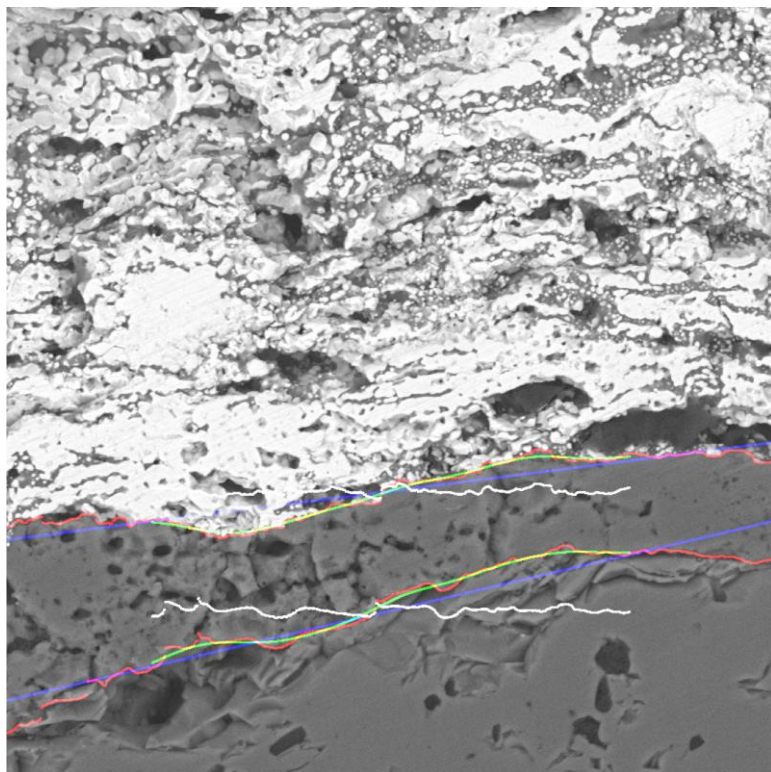
# Applications



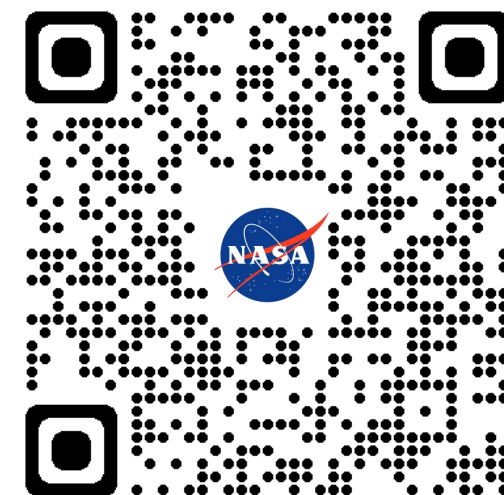
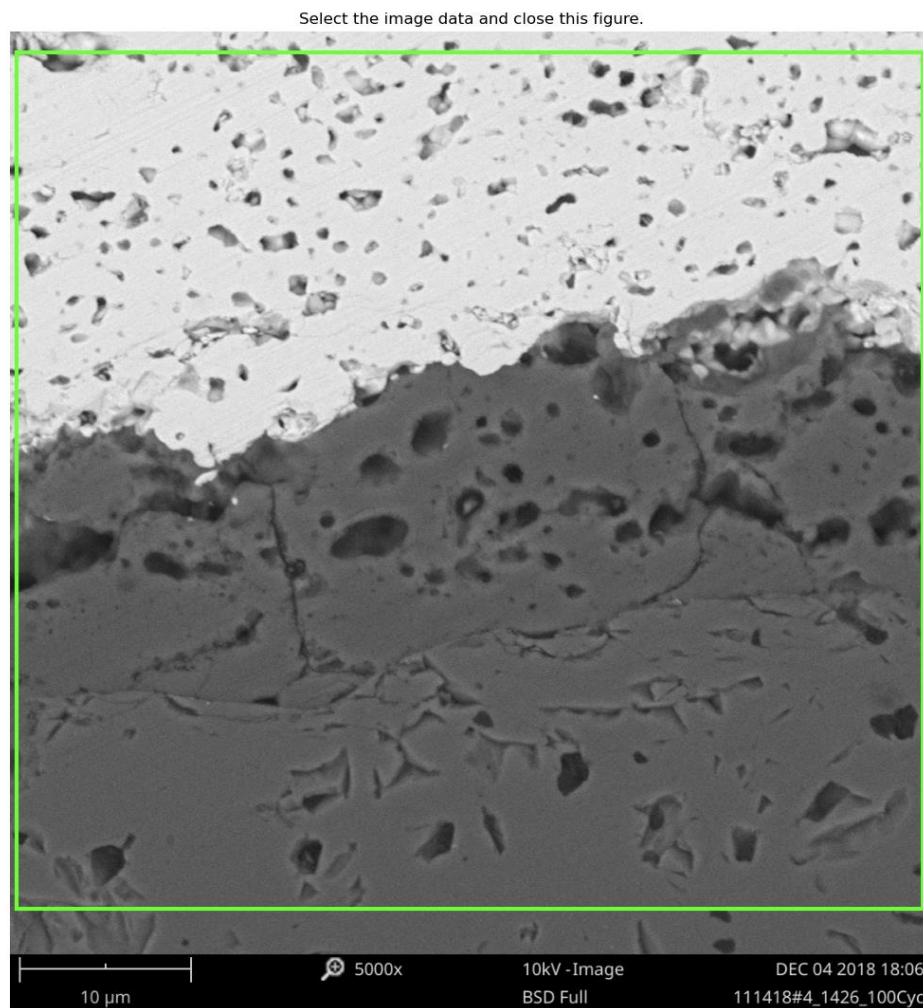
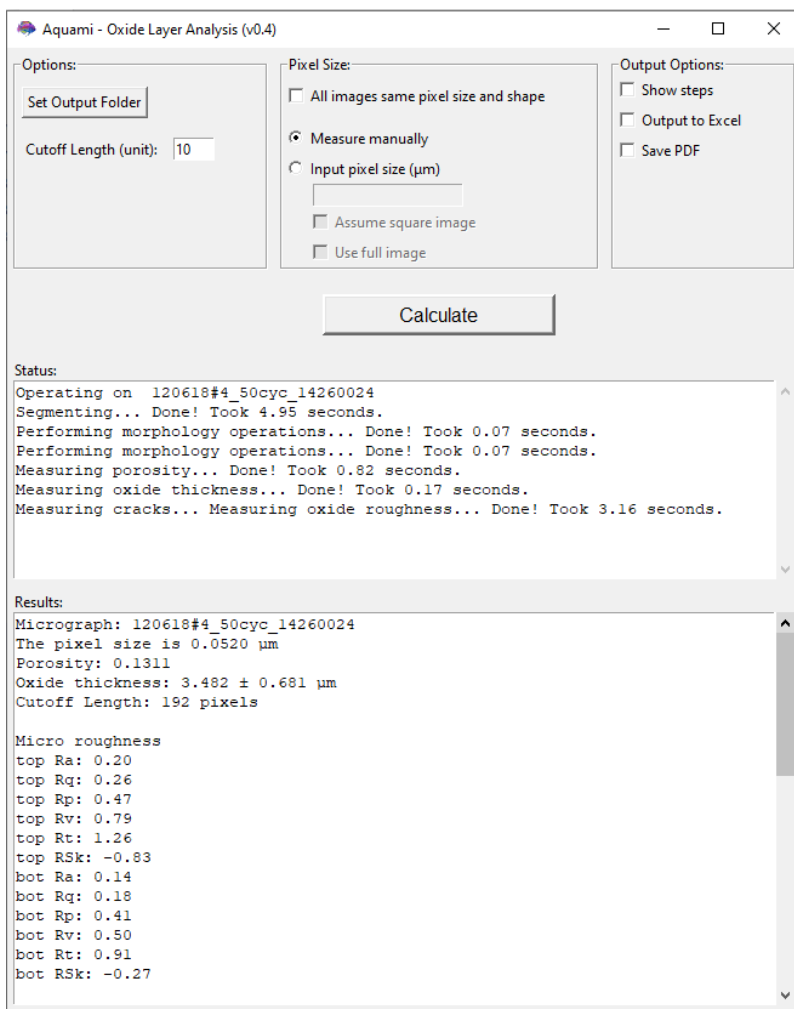
# Applications



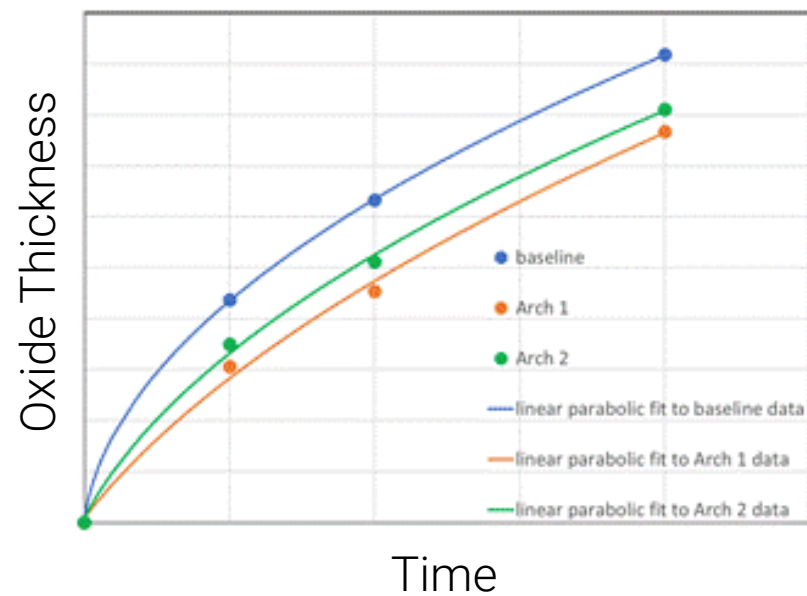
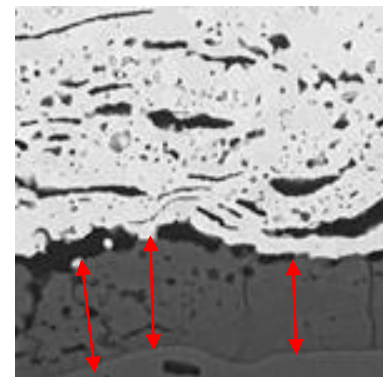
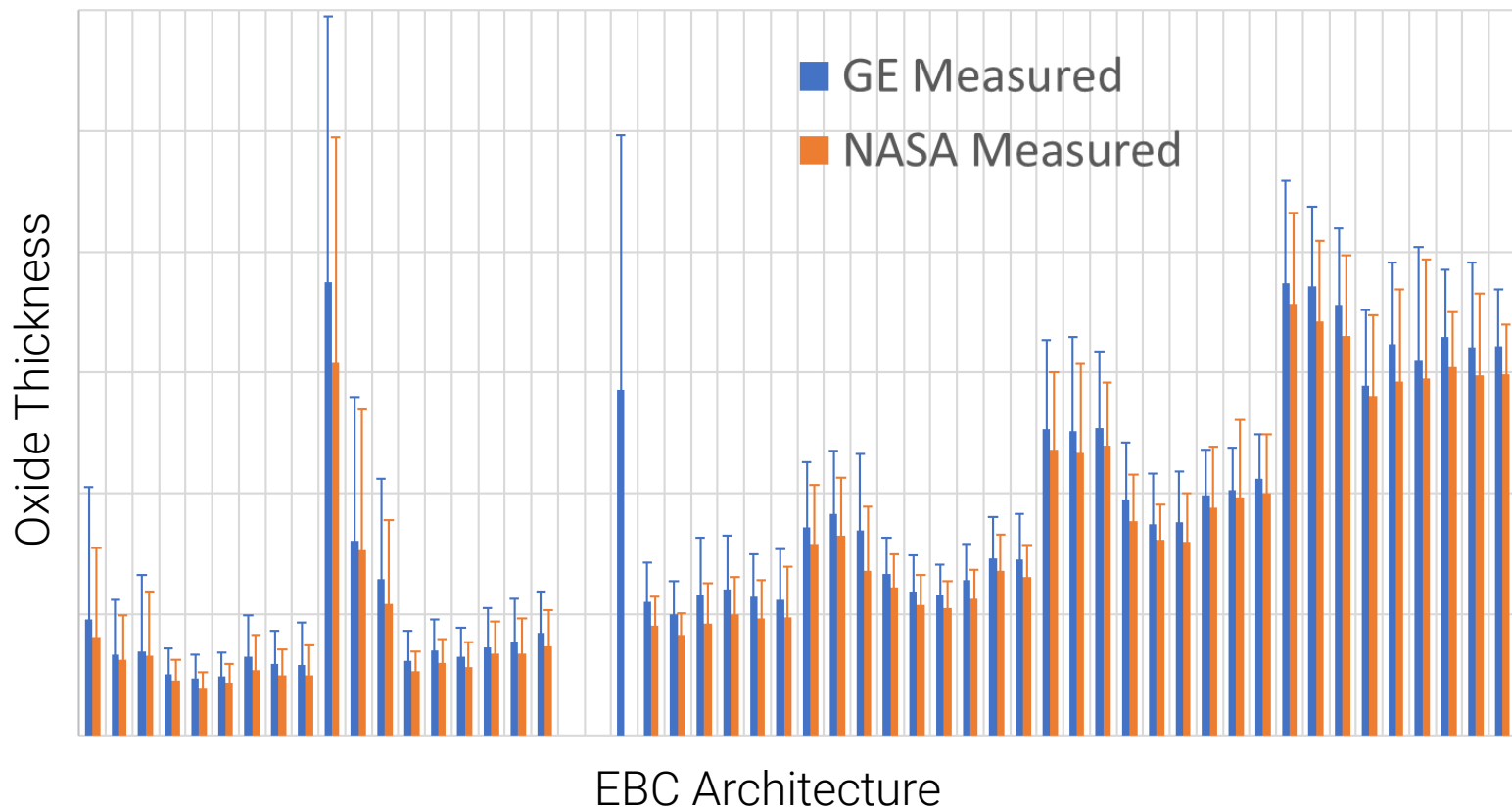
# Applications



## Open-Source Software GUI

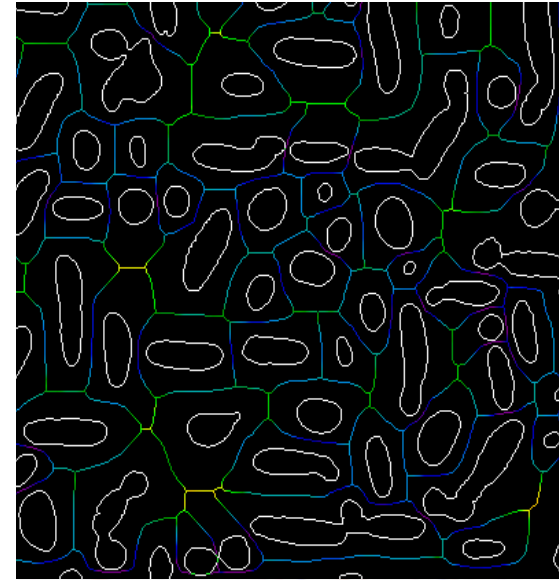
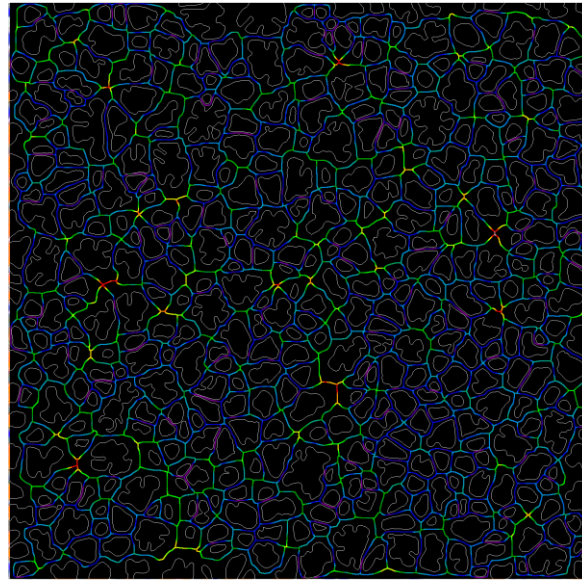
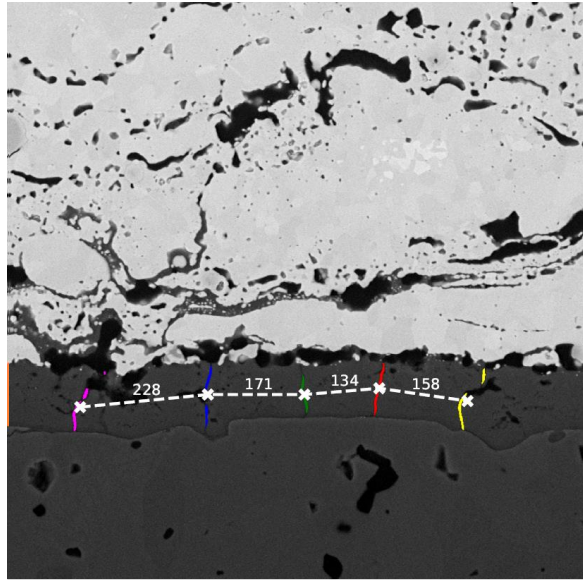


# Applications

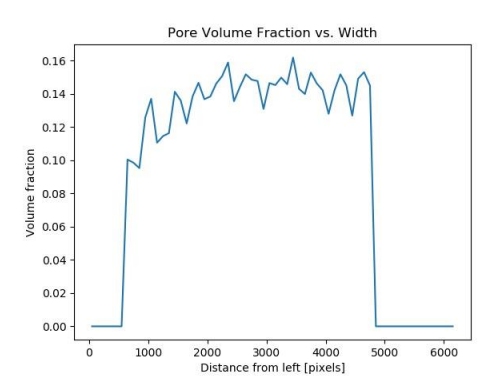
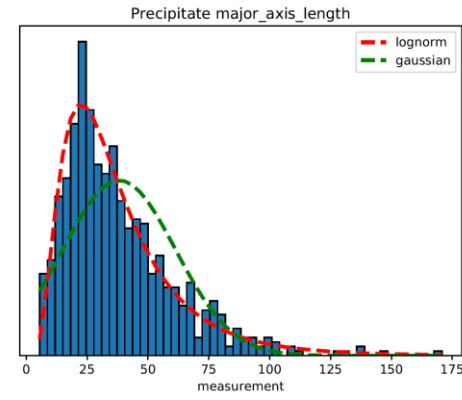
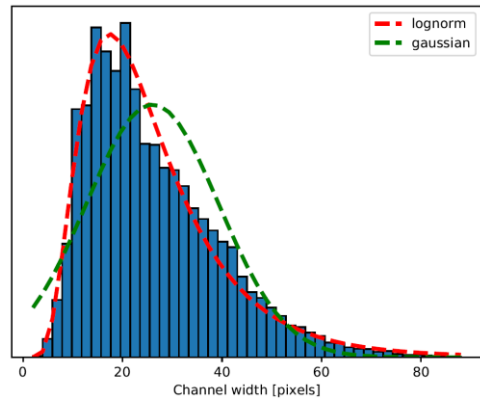
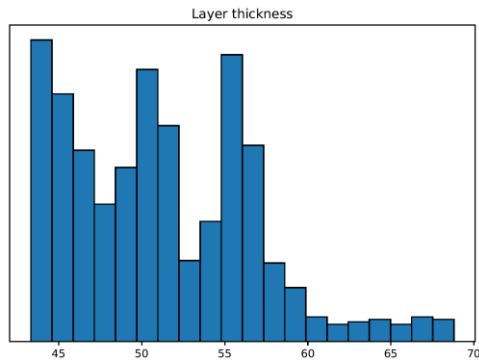




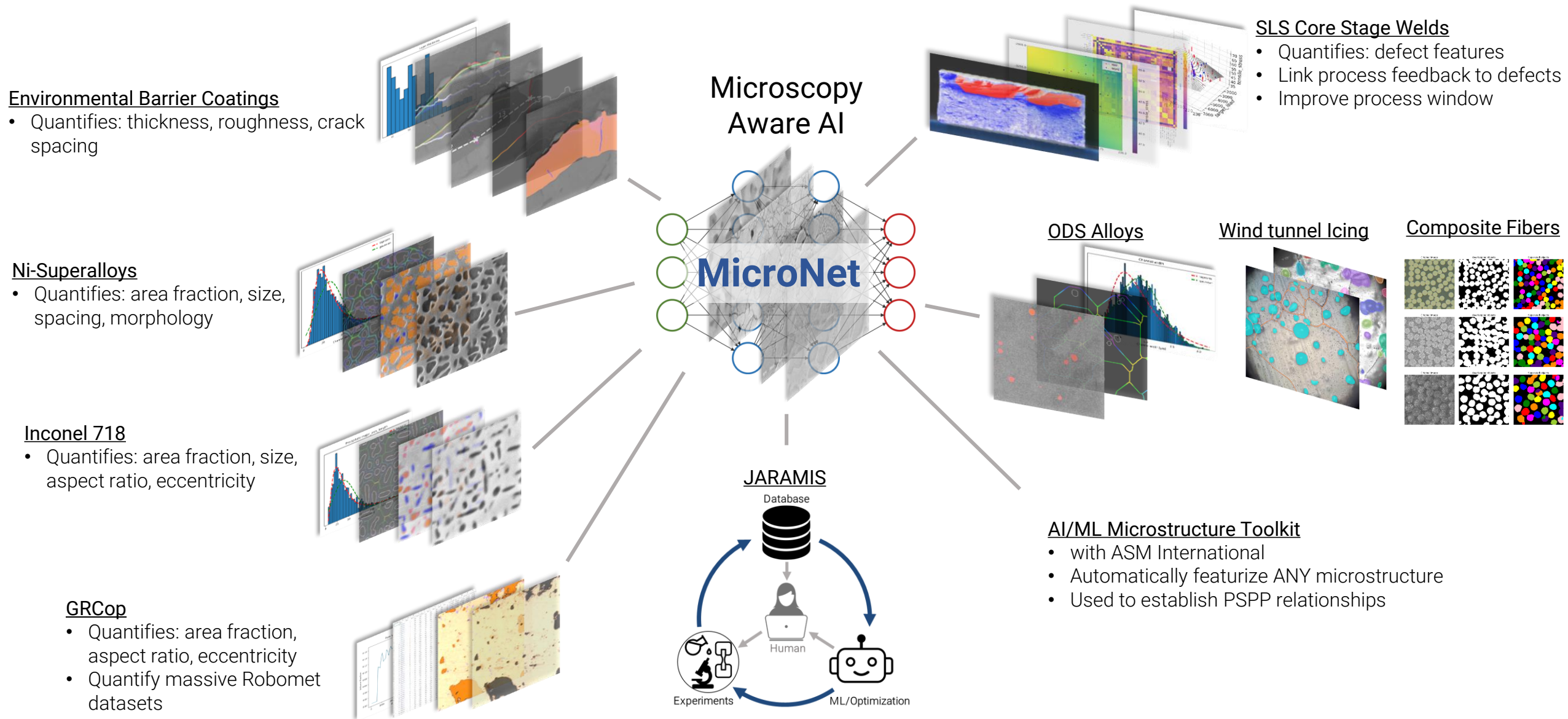
# Applications



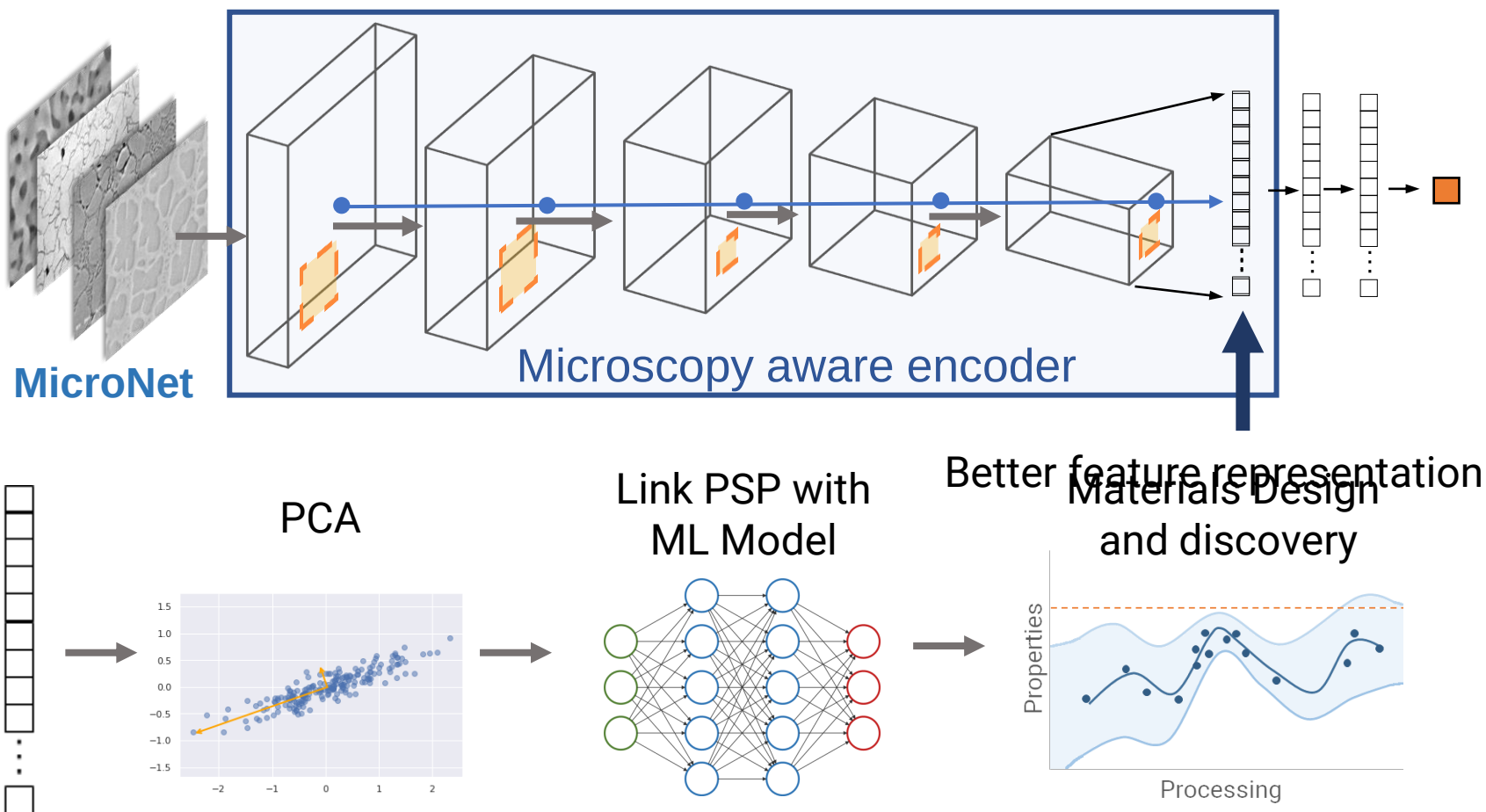
|    | A  | B         | C                        | D      | E      | F    | G         | H          | I          | J      | K            | L        | M        | N        | O        |
|----|----|-----------|--------------------------|--------|--------|------|-----------|------------|------------|--------|--------------|----------|----------|----------|----------|
|    | id | label     | centroid-centroid-bbox-0 | bbox-1 | bbox-2 | area | perimeter | major_axis | minor_axis | orient | eccentricity | e        |          |          |          |
| 1  | 0  | ISGRCop-1 | 1                        | 601    | 1289   | 600  | 1287      | 605        | 1292       | 15     | 12.48528     | 4.844241 | 4.0442   | -0.32175 | 0.550482 |
| 2  | 1  | ISGRCop-1 | 2                        | 603    | 1615   | 600  | 1629      | 609        | 1643       | 107    | 37.31371     | 14.72672 | 9.40229  | 1.40981  | 0.76906  |
| 3  | 2  | ISGRCop-1 | 3                        | 623    | 1520   | 600  | 1504      | 600        | 1534       | 983    | 133.9828     | 54.36489 | 23.78021 | 0.89989  | 0.89989  |
| 4  | 3  | ISGRCop-1 | 4                        | 605    | 1984   | 600  | 1973      | 615        | 1998       | 266    | 68.42031     | 23.36217 | 15.65205 | -1.54182 | 0.742385 |
| 5  | 4  | ISGRCop-1 | 5                        | 791    | 2222   | 600  | 2095      | 1007       | 2399       | 25384  | 2140.807     | 555.1083 | 120.2401 | 0.462952 | 0.976259 |
| 6  | 5  | ISGRCop-1 | 6                        | 600    | 2341   | 600  | 2339      | 602        | 2345       | 11     | 11.20711     | 6.410748 | 1.96494  | -1.51743 | 0.951888 |
| 7  | 6  | ISGRCop-1 | 7                        | 607    | 2933   | 600  | 2922      | 615        | 2950       | 302    | 76.29427     | 29.51659 | 14.64479 | 1.108884 | 0.871881 |
| 8  | 7  | ISGRCop-1 | 8                        | 671    | 3003   | 600  | 2974      | 755        | 3029       | 5144   | 453.8478     | 155.4692 | 45.61201 | -0.03779 | 0.955995 |
| 9  | 8  | ISGRCop-1 | 9                        | 601    | 1097   | 601  | 1096      | 603        | 1099       | 4      | 4.62132      | 2.828427 | 1.732051 | 1.570796 | 0.790569 |
| 10 | 9  | ISGRCop-1 | 10                       | 602    | 2329   | 601  | 2327      | 604        | 2332       | 5      | 5.414214     | 6.107531 | 1.047887 | 1.170957 | 0.985171 |
| 11 | 10 | ISGRCop-1 | 11                       | 606    | 2486   | 602  | 2478      | 613        | 2495       | 93     | 45.24874     | 16.90973 | 8.328791 | 1.265792 | 0.873462 |
| 12 | 11 | ISGRCop-1 | 12                       | 806    | 3340   | 604  | 3251      | 1026       | 3449       | 30725  | 1893.257     | 465.7336 | 157.8169 | 0.17195  | 0.940338 |
| 13 | 12 | ISGRCop-1 | 13                       | 608    | 1325   | 606  | 1324      | 611        | 1328       | 18     | 12.82843     | 5.258738 | 4.268749 | 0        | 0.584013 |
| 14 | 13 | ISGRCop-1 | 14                       | 614    | 3104   | 606  | 3098      | 622        | 3114       | 160    | 49.45584     | 18.69312 | 11.46851 | 0.03229  | 0.709883 |
| 15 | 14 | ISGRCop-1 | 15                       | 612    | 2382   | 609  | 2376      | 617        | 2390       | 52     | 33.55635     | 15.66732 | 4.693847 | 1.548764 | 0.954067 |
| 16 | 15 | ISGRCop-1 | 16                       | 614    | 2782   | 609  | 2777      | 620        | 2789       | 92     | 33.78899     | 12.18298 | 9.712257 | -1.10121 | 0.601543 |
| 17 | 16 | ISGRCop-1 | 17                       | 611    | 1117   | 610  | 1116      | 614        | 1119       | 8      | 7.658584     | 3.464102 | 2.828427 | 0        | 0.57775  |
| 18 | 17 | ISGRCop-1 | 18                       | 615    | 1742   | 613  | 1741      | 618        | 1746       | 19     | 13.65685     | 5.127073 | 4.712757 | -0.20933 | 0.940486 |
| 19 | 18 | ISGRCop-1 | 19                       | 651    | 3917   | 613  | 3860      | 678        | 3973       | 2050   | 346.4691     | 128.6058 | 35.77718 | 1.06904  | 0.960525 |
| 20 | 19 | ISGRCop-1 | 20                       | 614    | 1429   | 614  | 1429      | 617        | 1432       | 6      | 6.242641     | 3.126944 | 2.309401 | -0.7834  | 0.6742   |
| 21 | 20 | ISGRCop-1 | 21                       | 622    | 1234   | 615  | 1227      | 631        | 1244       | 213    | 51.45584     | 17.31964 | 15.6594  | -1.11228 | 0.423504 |
| 22 | 21 | ISGRCop-1 | 22                       | 618    | 2752   | 615  | 2746      | 622        | 2758       | 64     | 28.72792     | 11.83033 | 6.876038 | -1.31316 | 0.834064 |
| 23 | 22 | ISGRCop-1 | 23                       | 618    | 3214   | 618  | 3214      | 620        | 3216       | 2      | 0            | 2.828427 | 0        | -0.7834  | 1        |
| 24 | 23 | ISGRCop-1 | 24                       | 622    | 4328   | 618  | 4321      | 630        | 4335       | 66     | 41.2132      | 16.84038 | 10.06631 | -1.20992 | 0.801875 |
| 25 | 24 | ISGRCop-1 | 25                       | 621    | 2283   | 619  | 2281      | 625        | 2286       | 23     | 15.07181     | 5.026478 | 0.381184 | 0.501706 |          |
| 26 | 25 | ISGRCop-1 | 26                       | 621    | 1473   | 620  | 1473      | 625        | 1476       | 18     | 13.65685     | 5.276229 | 4.361835 | -0.19546 | 0.562649 |
| 27 | 26 | ISGRCop-1 | 27                       | 627    | 3524   | 626  | 3523      | 630        | 3528       | 11     | 11.24264     | 5.09304  | 2.855525 | 1.155988 | 0.764097 |
| 28 | 27 | ISGRCop-1 | 28                       | 632    | 3032   | 628  | 3029      | 637        | 3037       | 59     | 25.89949     | 9.380872 | 8.024764 | 0.314584 | 0.517704 |
| 29 | 28 | ISGRCop-1 | 29                       | 629    | 3083   | 629  | 3081      | 630        | 3082       | 2      | 0            | 0        | 0        | 1.570796 | 1        |
| 30 | 29 | ISGRCop-1 | 30                       | 636    | 3043   | 633  | 3040      | 641        | 3048       | 53     | 24.48528     | 3.80557  | 8.072153 | -0.7225  | 0.268785 |
| 31 | 30 | ISGRCop-1 | 31                       | 637    | 2393   | 634  | 2389      | 642        | 2398       | 57     | 25.31371     | 9.653777 | 7.493182 | -1.12026 | 0.830497 |
| 32 | 31 | ISGRCop-1 | 32                       | 639    | 1300   | 637  | 1296      | 643        | 1304       | 26     | 16.48328     | 5.89992  | 5.600679 | -1.29547 | 0.314466 |
| 33 | 32 | ISGRCop-1 | 33                       | 639    | 1372   | 638  | 1372      | 641        | 1375       | 8      | 7.414214     | 1.464102 | 2.738613 | -0.7834  | 0.612372 |
| 34 | 33 | ISGRCop-1 | 34                       | 640    | 1193   | 639  | 1191      | 643        | 1196       | 9      | 8.414214     | 0.253888 | 1.850618 | -0.7834  | 0.953483 |
| 35 | 34 | ISGRCop-1 | 35                       | 645    | 1867   | 643  | 1861      | 648        | 1872       | 39     | 21.65685     | 9.477889 | 5.234648 | 1.491802 | 0.833617 |
| 36 | 35 | ISGRCop-1 | 36                       | 641    | 4345   | 643  | 4345      | 645        | 4347       | 4      | 4            | 0        | 0        | 0.769398 | 0        |
| 37 | 36 | ISGRCop-1 | 37                       | 657    | 2724   | 644  | 2666      | 1074       | 2800       | 26892  | 1857.653     | 457.7142 | 112.1925 | -0.04046 | 0.969273 |
| 38 | 37 | ISGRCop-1 | 38                       | 647    | 1016   | 646  | 1015      | 649        | 1019       | 10     | 8.828427     | 4.38178  | 2.683282 | -1.10715 | 0.790569 |
| 39 | 38 | ISGRCop-1 | 39                       | 673    | 4246   | 646  | 4221      | 699        | 4270       | 1157   | 169.131      | 65.10788 | 25.27602 | -0.88376 | 0.921567 |
| 40 | 39 | ISGRCop-1 | 40                       | 649    | 3993   | 647  | 3993      | 652        | 3995       | 8      | 8.828427     | 5.444425 | 2.252495 | -0.0883  | 0.510318 |
| 41 | 40 | ISGRCop-1 | 41                       | 649    | 2062   | 648  | 2060      | 652        | 2065       | 14     | 11.65685     | 4.505941 | 3.961881 | 0.847576 | 0.476347 |
| 42 | 41 | ISGRCop-1 | 42                       | 651    | 4008   | 649  | 4004      | 658        | 4014       | 64     | 28.14214     | 9.57109  | 8.517354 | -1.30442 | 0.452047 |
| 43 | 42 | ISGRCop-1 | 43                       | 651    | 1509   | 651  | 1508      | 654        | 1511       | 7      | 6.828427     | 3.023716 | 2.799417 | 1.570796 | 0.377964 |
| 44 | 43 | ISGRCop-1 | 44                       | 651    | 1912   | 651  | 1912      | 652        | 1914       | 2      | 0            | 0        | 0        | 1.570796 | 1        |
| 45 | 44 | ISGRCop-1 | 45                       | 655    | 2286   | 651  | 2282      | 660        | 2292       | 65     | 28.14214     | 9.34746  | 8.82033  | 1.374312 | 0.321237 |
| 46 | 45 | ISGRCop-1 | 46                       | 705    | 1113   | 652  | 1070      | 705        | 1161       | 4269   | 512.4163     | 126.7348 | 62.60873 | 0.795239 | 0.869404 |
| 47 | 46 | ISGRCop-1 | 47                       | 654    | 3093   | 653  | 3092      | 656        | 3096       | 11     | 9.414214     | 6.346133 | 1.067706 | -1.30776 | 0.708484 |
| 48 | 47 | ISGRCop-1 | 48                       | 667    | 3746   | 653  | 3676      | 7100       | 3888       | 44587  | 1871.131     | 511.9471 | 167.1734 | 0.00007  | 0.844878 |



# Applications



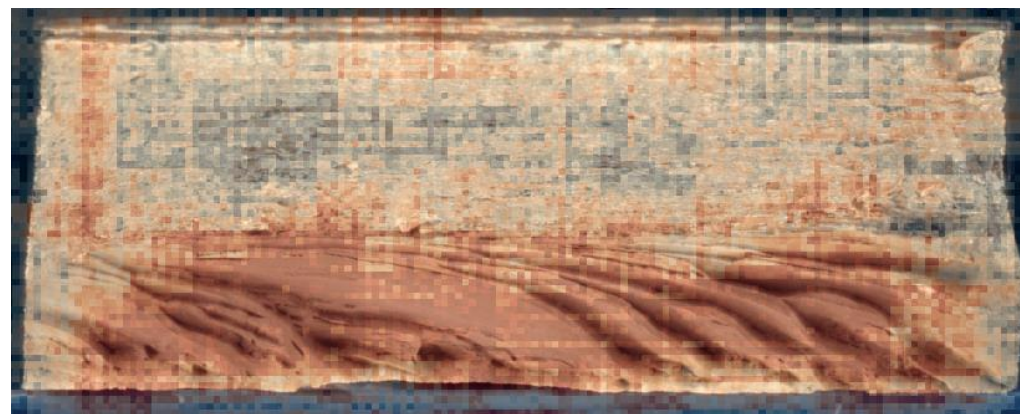
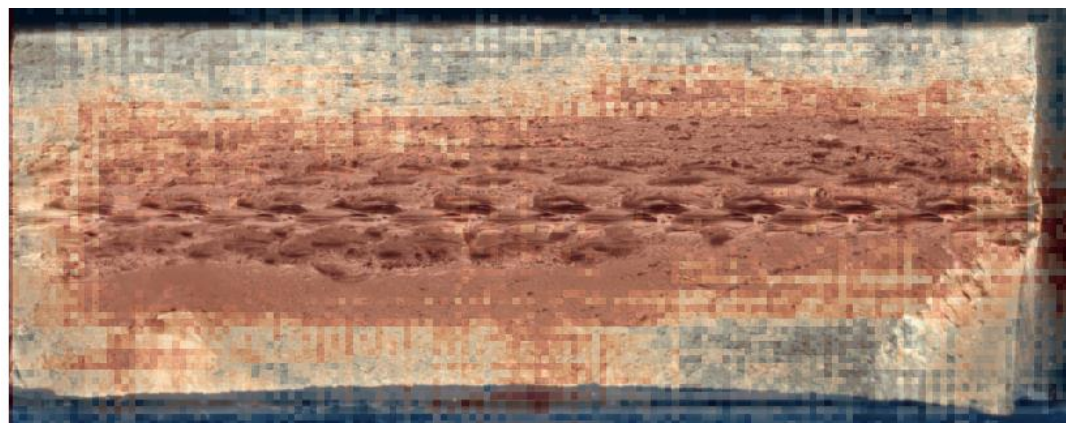
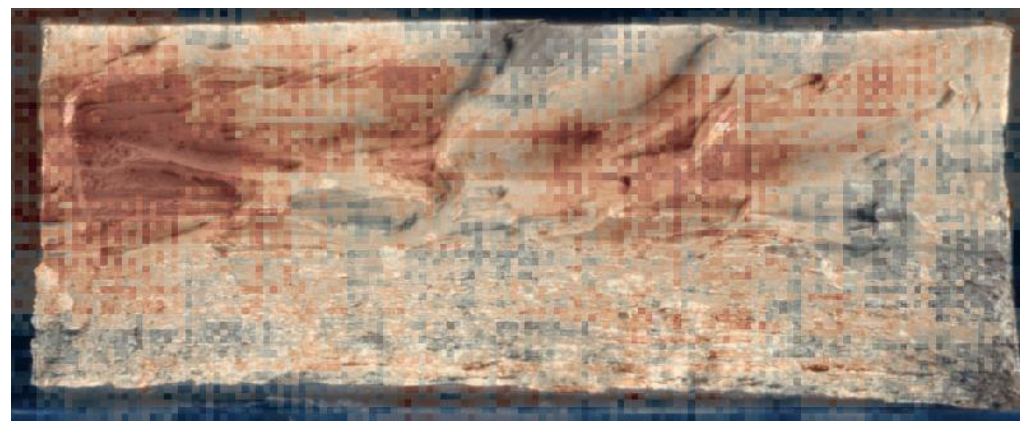
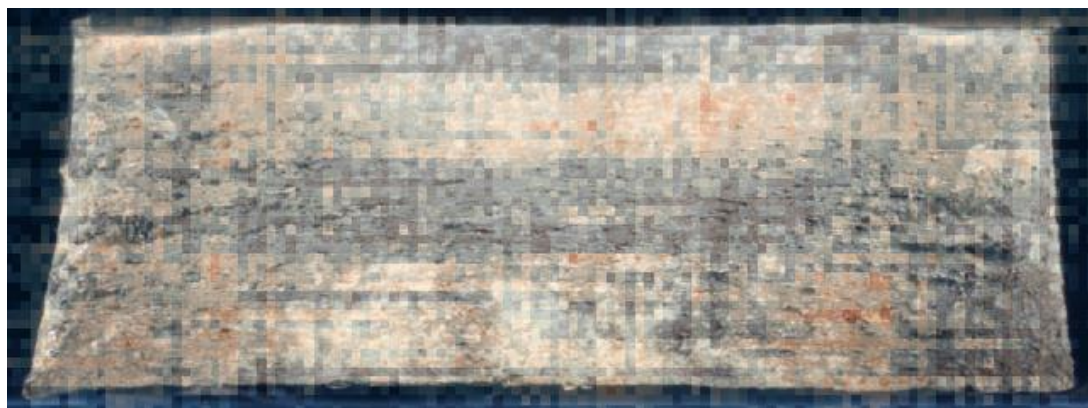
# Applications



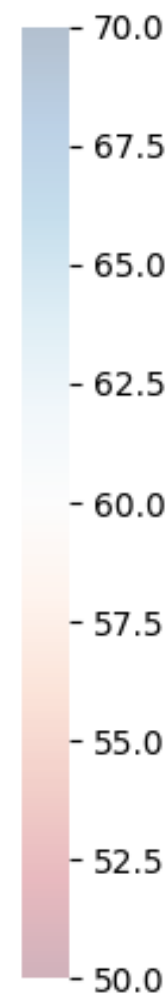
1. R. Noraas, et al., "Structural Material Property Tailoring Using Deep Neural Networks," in *AIAA Scitech 2019 Forum*, 2019, p. 1703.
2. M. Larmuseau, et al., "Compact representations of microstructure images using triplet networks," *npj Comput. Mater.*, vol. 6, no. 1, 2020
3. B. L. DeCost, et al., "High throughput quantitative metallography for complex microstructures using deep learning: A case study in ultrahigh carbon steel," *Microsc. Microanal.*, vol. 25, 2019

# Applications

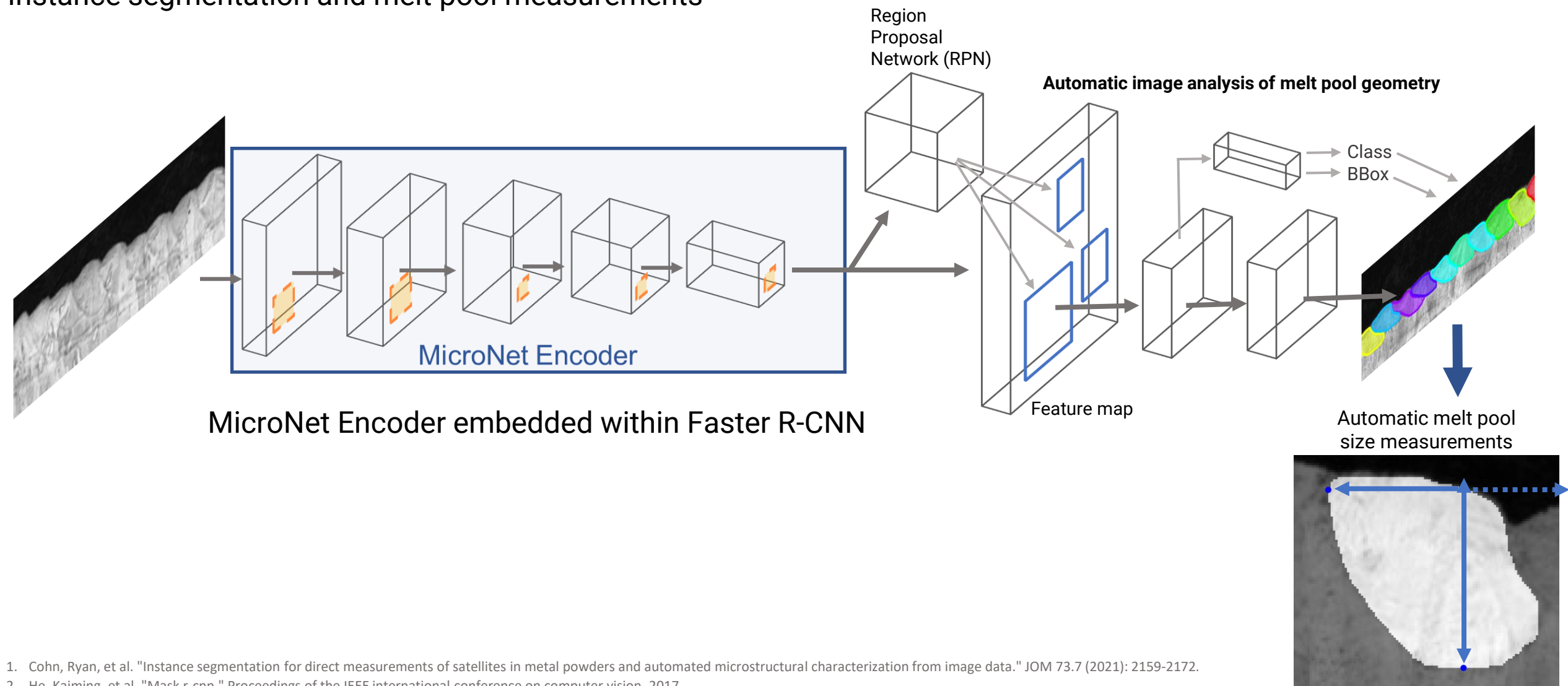
## Direct regression and patch prediction



Property  
(Normalized)



## Instance segmentation and melt pool measurements



1. Cohn, Ryan, et al. "Instance segmentation for direct measurements of satellites in metal powders and automated microstructural characterization from image data." JOM 73.7 (2021): 2159-2172.
2. He, Kaiming, et al. "Mask r-cnn." Proceedings of the IEEE international conference on computer vision. 2017.

- **General microstructure aware pre-trained encoders**
  - Higher accuracy with less training data
  - More robust to changes in imaging and sample conditions
- Automatically extract microstructure features to establish processing-structure-processing relationships
- Can easily be applied to any computer vision architecture that utilizes pre-trained CNNs
- All code and models are open-source and easy to use with examples

## Code



