Deep Learning for Characterization of Deformation Induced Damage

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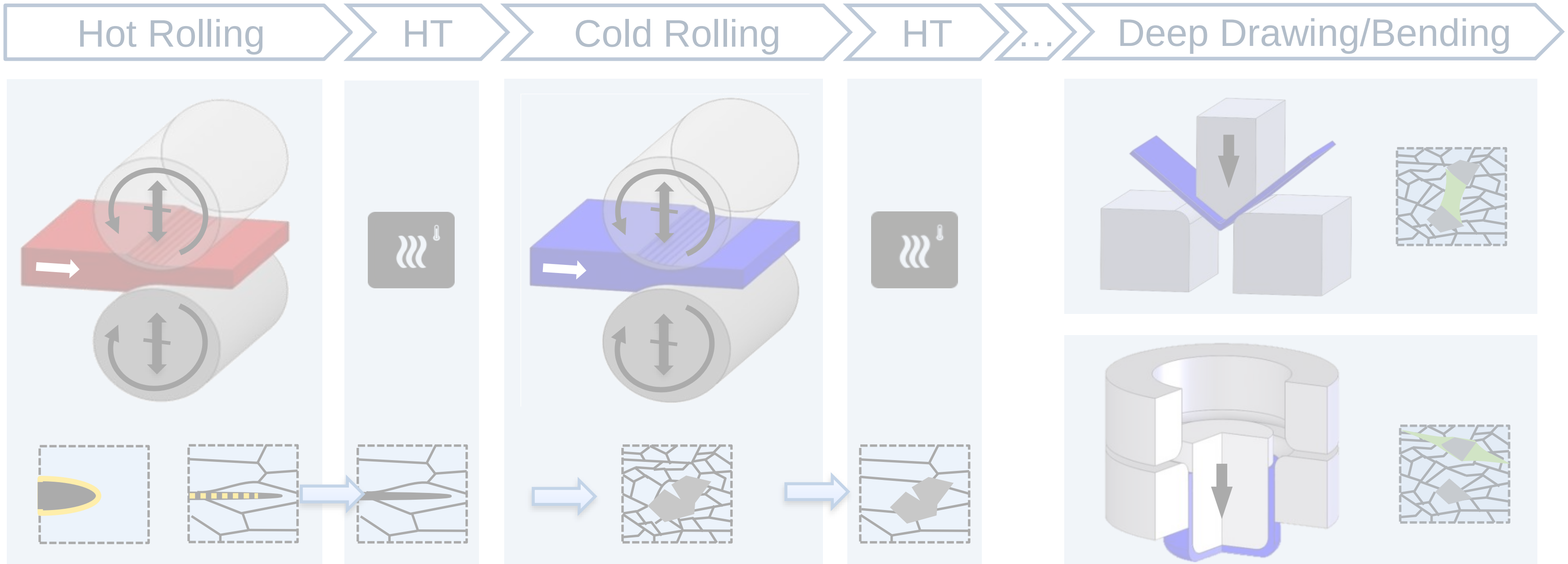
TMS 2021 – virtual conference

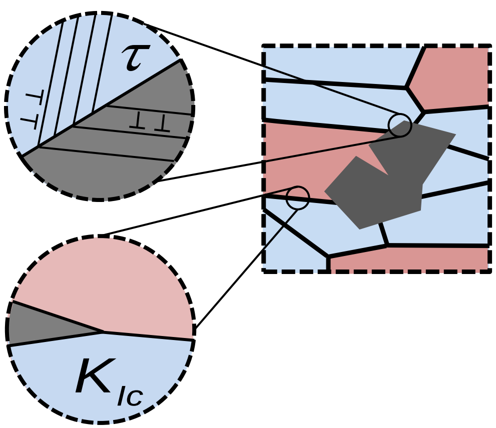
Why Steel?

One of our most versatile materials.

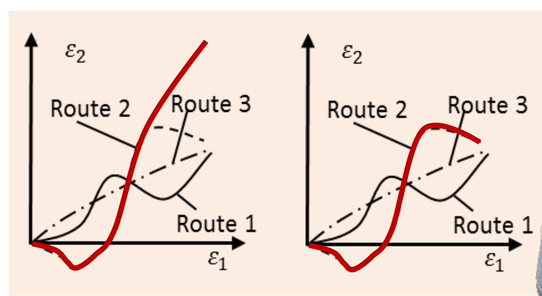
Important for industrial applications:
Dual Phase steel (e.g. DP800)



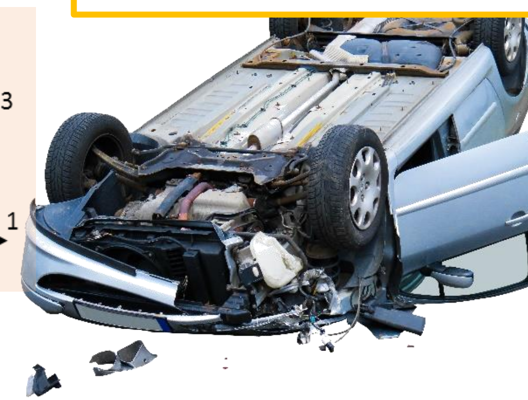
Damage Mechanisms

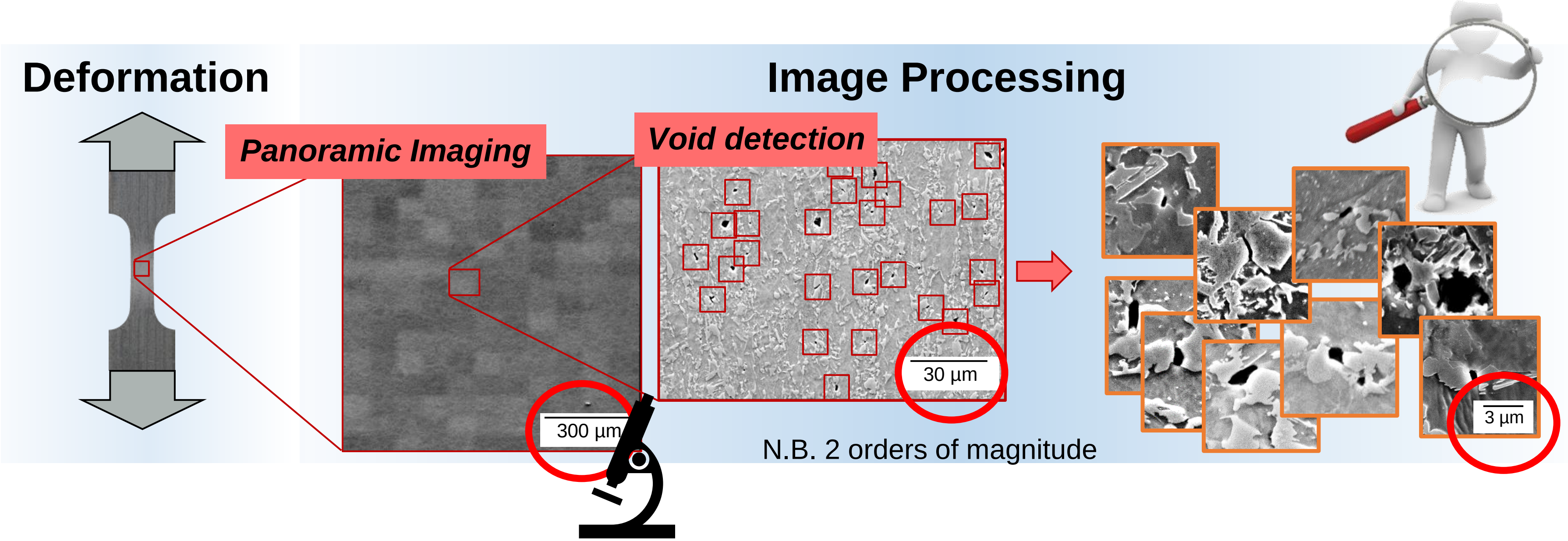


Better Processes

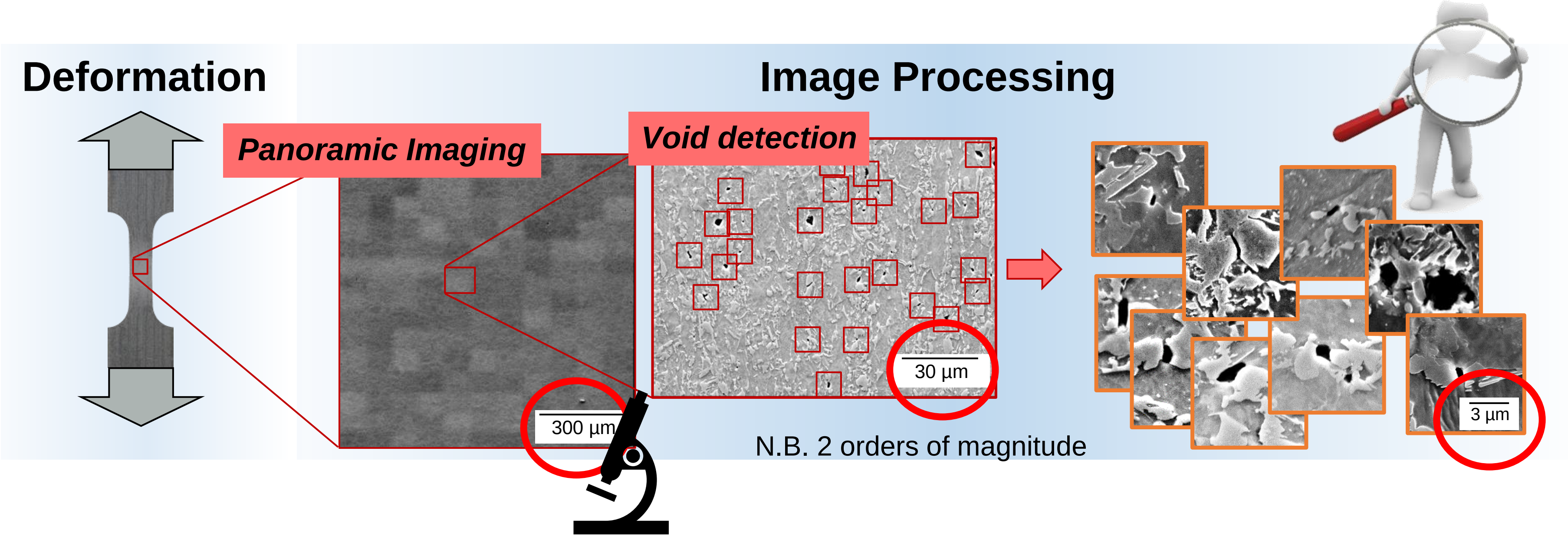


Better Materials





apply stress on material sample → electron microscope imaging → Damage localization → manual image analysis

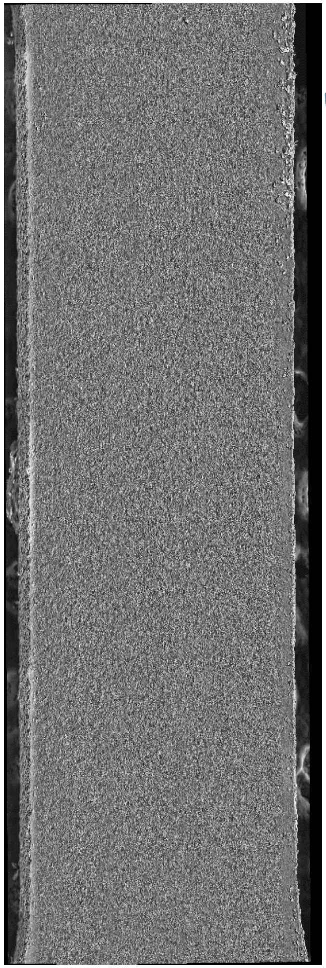


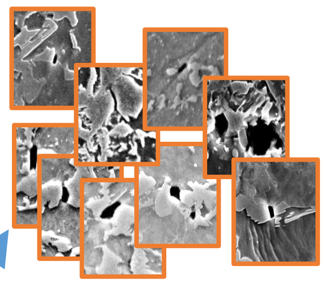
apply stress on material sample → electron microscope imaging → Damage localization → manual image analysis

- Detailed understanding of individual damage sites & mechanisms
- Manual approach does not allow statistical analysis

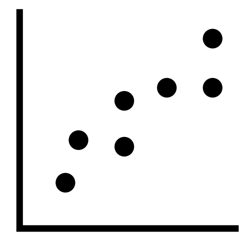
→ Automate image analysis with Deep Learning

Key Steps in Automated Damage Analysis





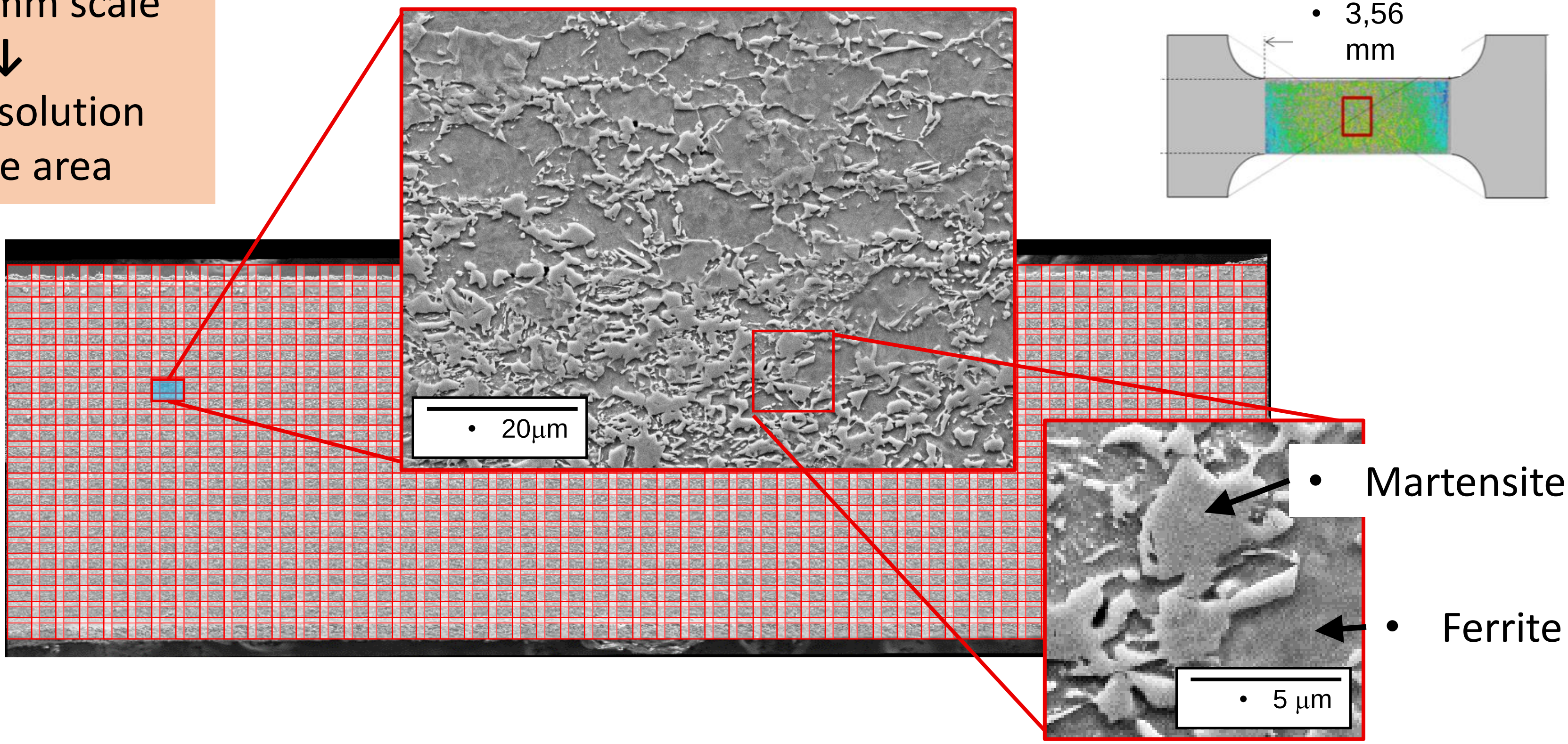
~10,000 images



Obtain high-res panoramic image → Automated damage localization → Deep learning: Damage ID → Statistical Analysis

Challenge I: Many Damage Sites

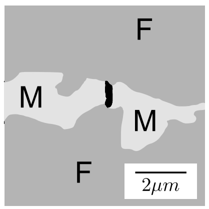
Heterogeneous at
< µm – mm scale
↓
High resolution
+ large area



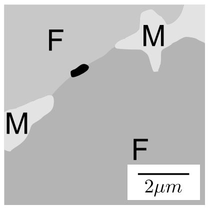
High-res panoramic image of a large sample space
→ Handle many images

- OK for PoC
- Setup data infrastructure for continued analysis (Image + Metadata) (e.g., Mongo DB)

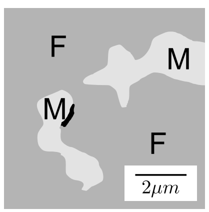
Supervised learning: Require labelled images – definition of semantic classes?



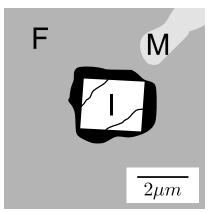
Martensite Cracking



Grain Boundary Decohesion

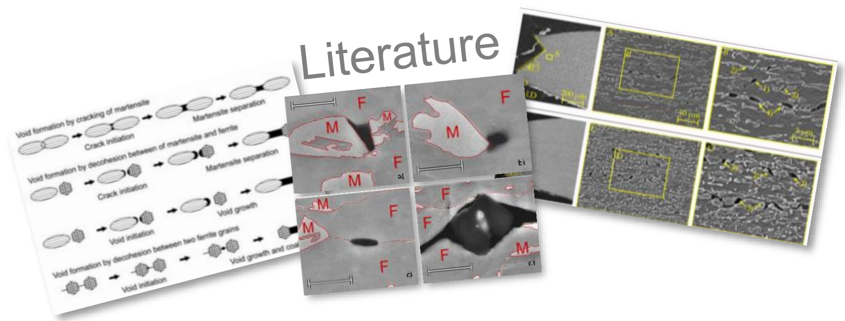


Interface Decohesion



Inclusion

Step 1: Relevant Literature



Hoefnagels, J.P.M., et al. (2015) || J Mater Sci 50(21) 6882
Azuma, M. (2013) PhD thesis, TU Denmark || Heibel, S. et al. (2018) Materials 11, 761

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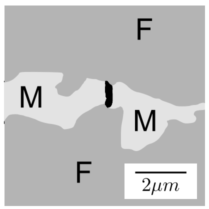

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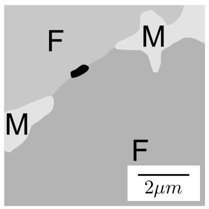

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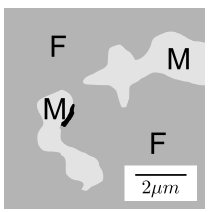

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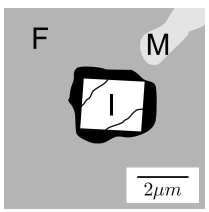

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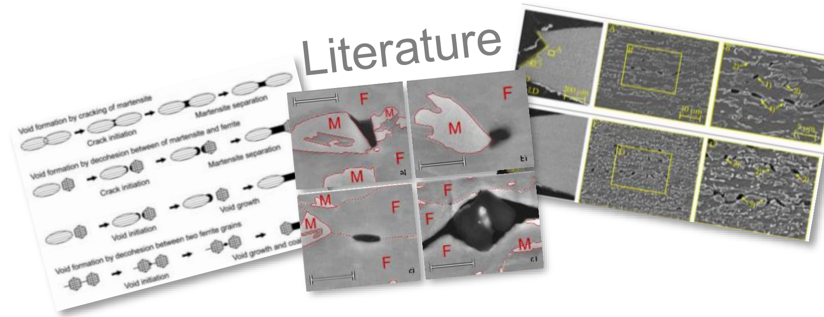

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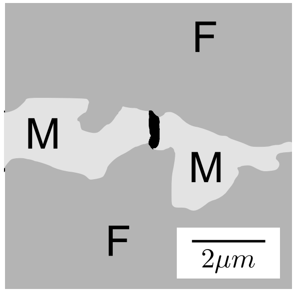
Step 2: Revise & Clarify Class Definitions

- Class definitions suitable for “clear cut” cases (what is normally looked at)
- Many “in-between” cases
    - Important for statistical analysis
    - Consolidate class labels with multiple experts

Challenge II: Semantic Classes



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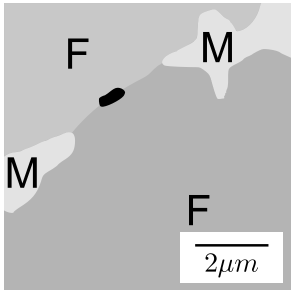
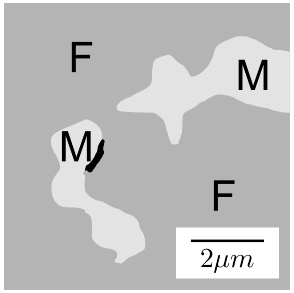
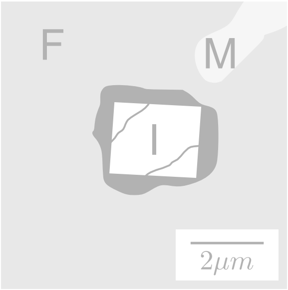


Grain Boundary Decohesion



Interface Decohesion



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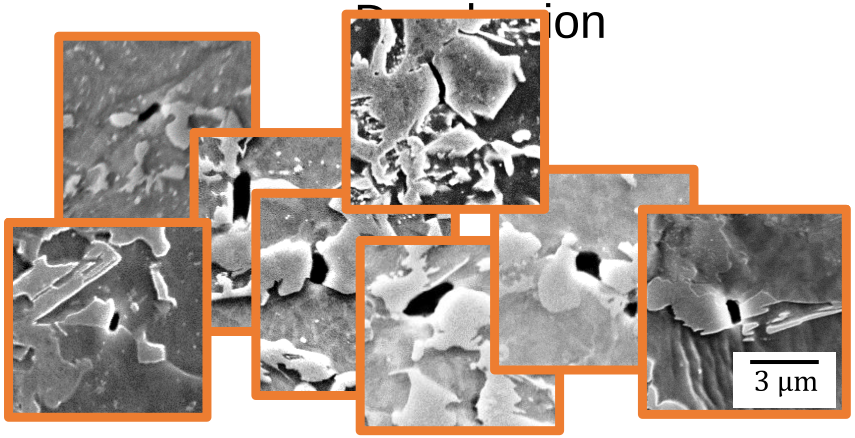
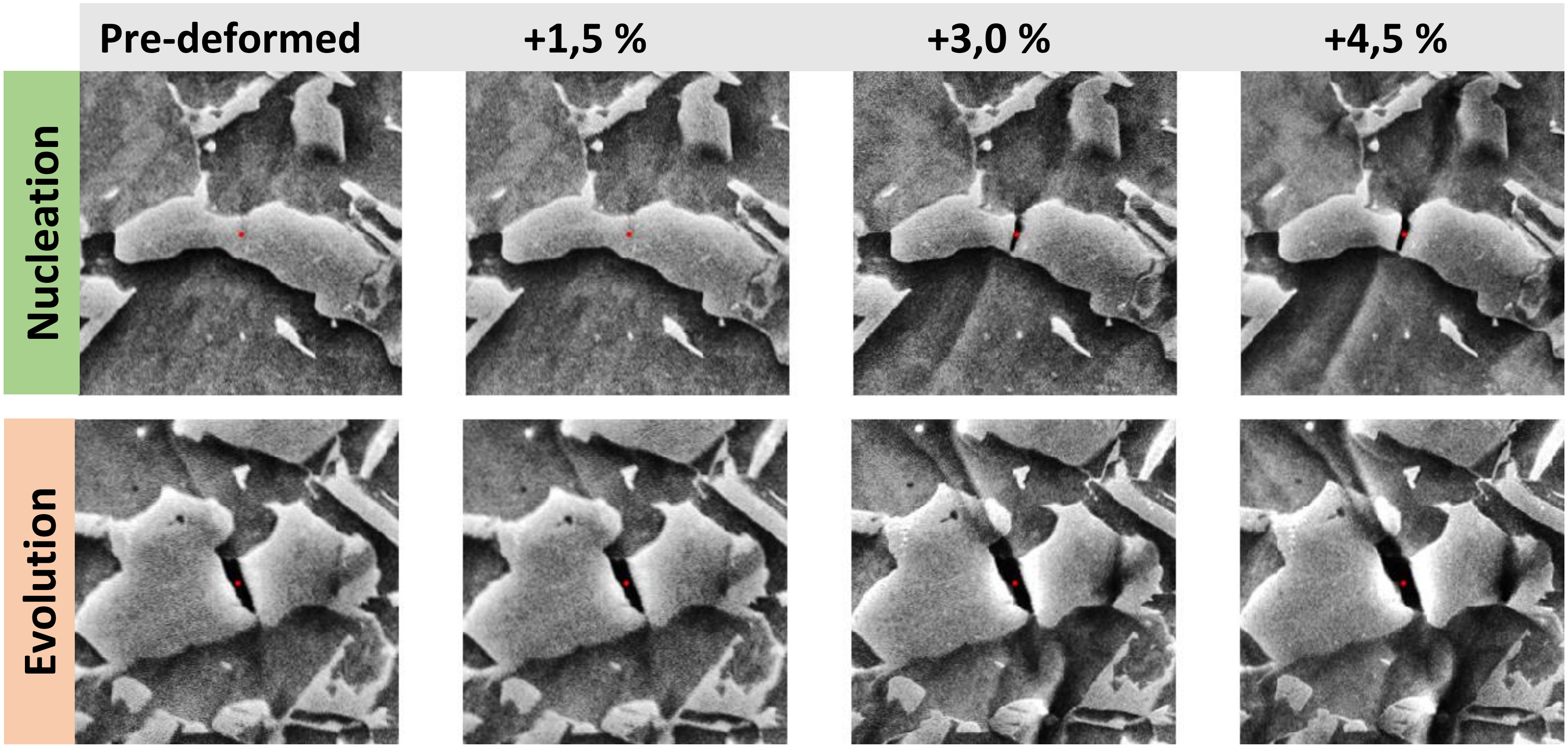


Panoramic imaging → big data

Kusche et al. (2019) PloS one 14 (5), e0216493

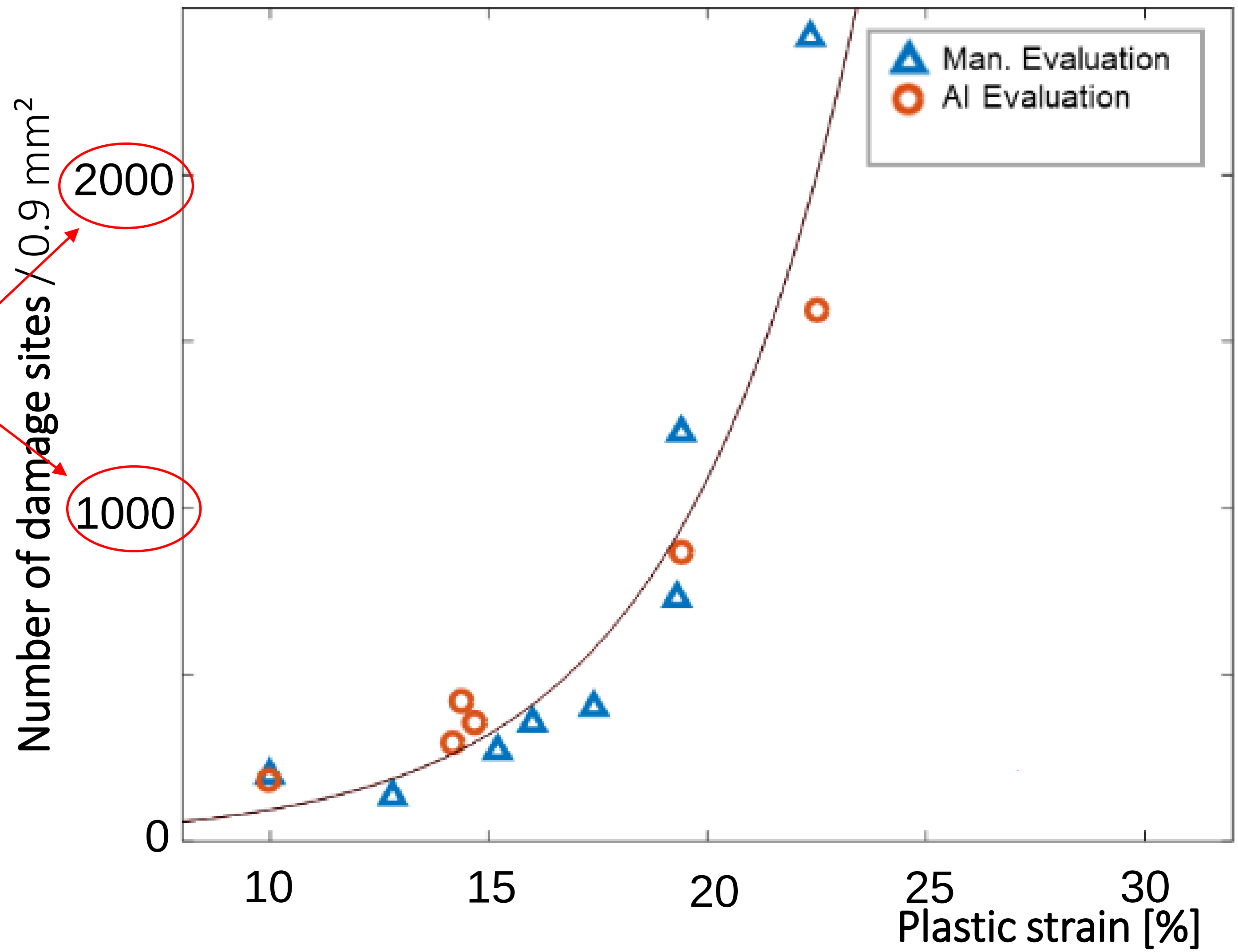
In-Situ Tracking: From Nucleation to Evolution



Kusche et al. (2019) PloS one 14 (5), e0216493

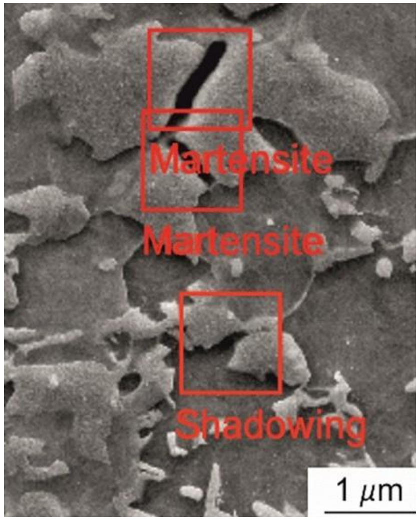
Compare Deep learning results with manual expert verification

N.B.:
large scale
verification



Kusche et al. (2019) PloS one 14 (5), e0216493

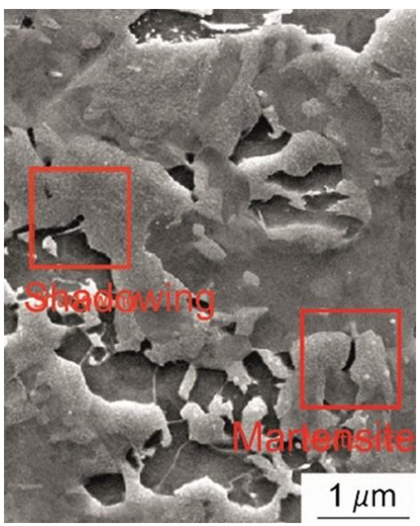
Challenge III: Image Artefacts

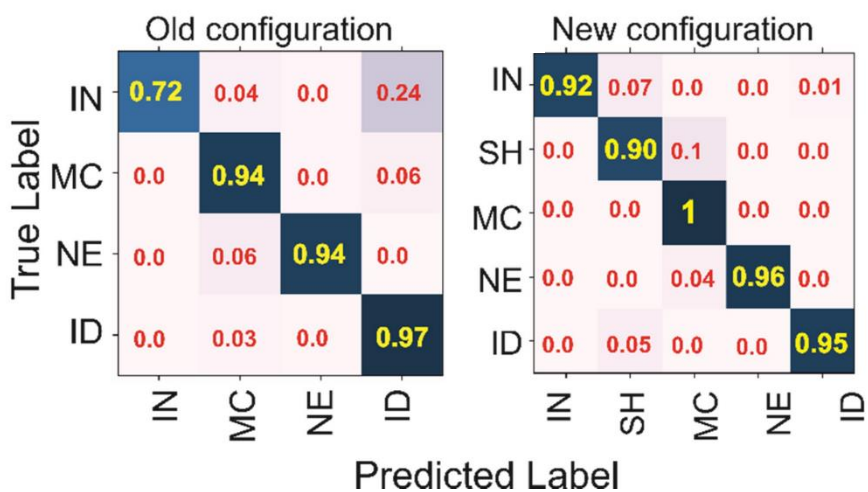


Imaging artifacts increase mis-classification

- In particular: shadows of e-beam on 3D sample structure
- Extend semantic classes: add artefact “SH” (shadow) as class
    - Significant increase in performance
    - So far: major artefact – but monitor for new preparations

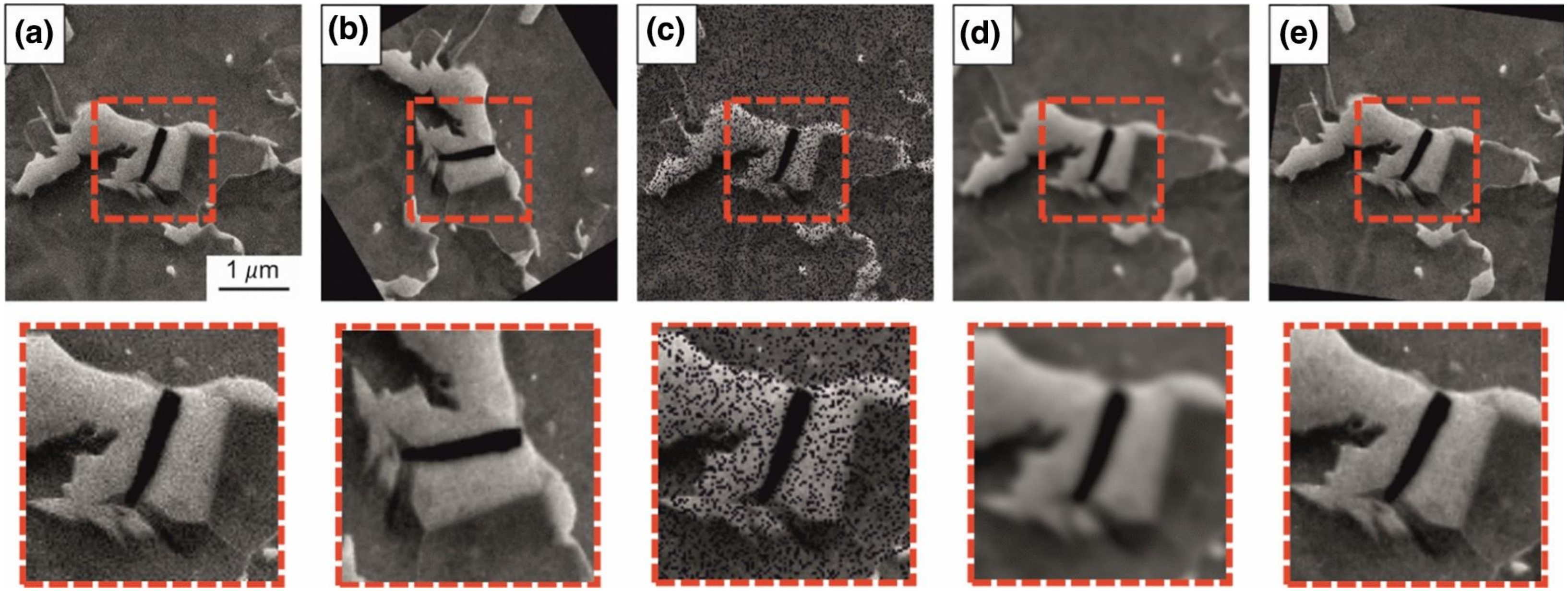
Data *doesn’t* speak for itself!





Supervised Learning:

- Requires labelled images *representative* of sample for inference.
- Costly to obtain: Manual work by experts
- Challenge for generalizability – example: uniaxial to biaxial stress
- Approach: image augmentation
    - Rotation, pixel dropout, blur, shear



Augmentations:
(a) original image, (b) random rotation, (c) random pixel dropout, (d) Gaussian blur, and (e) random shear.

S. Medghalchi, C. Kusche, E. Karimi, U. Kerzel, S. Korte-Kerzel (2020), *Damage Analysis in Dual Phase Steel Using Deep Learning: Transfer from Uniaxial to Biaxial Straining Conditions by Image Data Augmentation*, JOM (2020). DOI 10.1007/s11837-020-04404-0

Road Ahead: Data Handling

mongoDB®

Beyond PoC: Organize data systematically

Store data (images) *and* metadata:

- Date, time, location, sample ID
- Experimental conditions of imaging equipment
    - Microscope settings,
    - beam acceleration,
    - ….
- Sample details
    - Details about the sample, manufacturing process, …
    - Preparation prior to imaging (etching, ….)
    - …
- Image relationship
    - Original image as recorded
    - Image after enhancement
    - Stitched panorama
    - Identified image location (incl. location details)
    - …
- ….

No community-wide infrastructure available.

mongoDB seems promising candidate:

- Mature technology
- Open source
- Community to enterprise option
- Cloud scaling to planetary scale possible
- Connectors
- PyMongo for Python access

Supervised learning is the greatest thing (after sliced bread):

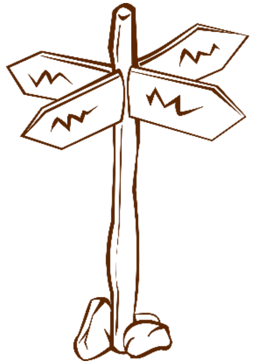
- Machine learning algorithm learns desired mapping: labelled images to label

- Semantic classes well defined:
  - Hand-crafted and verified by experts in the field
  - Artifacts can be included in well defined way

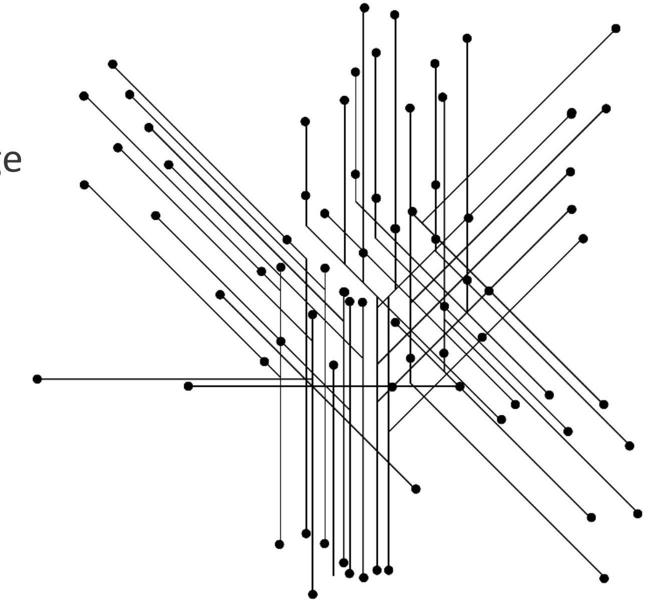
- Data doesn't speak for itself:
  - Verify semantic classes
  - Include expert knowledge in image labels

…. But: Doesn't scale
- New data need to be labelled manually
- Data labelling doesn't get much faster with time
- Additional people: expert training required.

→ explore further options:
Deep clustering, self-supervised, semi-supervised, semi-self supervised, contrastive learning, …



Potential Avenue: Clustering



Representation Learning + Clustering

1. Use deep convolutional neural networks (CNN) to extract image features
2. Use clustering (e.g. k-means) to group images into classes

- Little to no labelled data required

- CNN are not explainable –
  decision boundaries do not match well with expert analysis
- High and hard to control risk to learn artefacts instead of semantic classes.
- Number of clusters: free parameter

Examples:

- Deep Adaptive Clustering (J. Chang et al, ICCV 2017)
- DeepCluster (M. Caron et al., ECCV 2018, arXiv: 1807.05520)
- DeeperCluster (M. Caron et al. ICCV 2019, arXiv: 1905.01278)
- Deep Image Clustering With Spatial Transformer (Th. V. M. Souza et al., ICANN 2019, arXiv: 1902.05401)
- ClusterFit (X. Yan et al., IEEE/CVF CV 2020, arXiv: 1912.03330)
- SCAN (W. v. Gansbeke et al, ECCV 2020, arXiv: 2005.12320)
- Self-labelling via simultaneous clustering and representation learning (Y. Asano et al, ICLR 2020, arxiv: 1911.05371)

- In materials science: R. Cohn & E. Holms (2020), arXiv: 2007.08361)

Potential Avenue: Semi- / Self- Supervised Learning

Intuition: Reduce dependency on labelled images
Split training into two steps:

- Pre-train network with a suitable "pretext" task
- Fine-tune network with labelled images on actual task.

Idea:

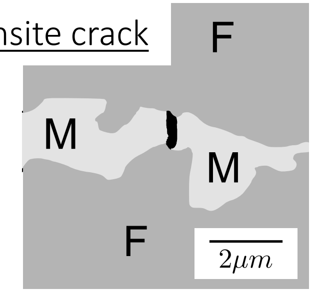
- Pretext task is something humans could do – but computers can do without human input
  - Pretext learns general representations
- Need much fewer labelled images once pretext task is trained
  - Downstream learns specifics for the actual task.

Challenges:

- Define a suitable pre-text for electron microscope imaging
  - Typically: colorization, position in image, fill a gap,…
  - Material science…?
- Networks at high risk to learn artefacts in pretext task
  - Scratches, blurs, watermarks, aberrations, …

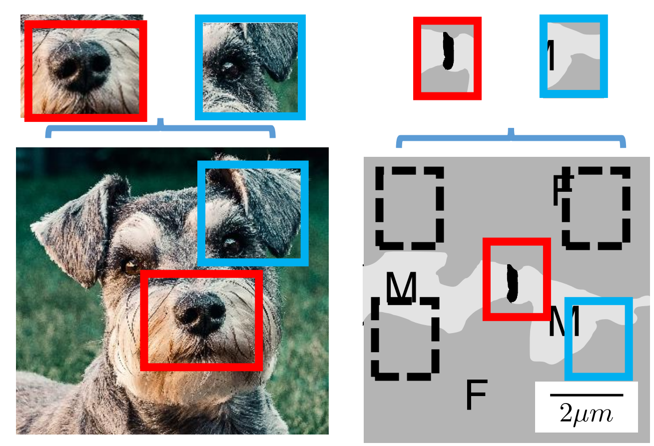
  (M. Minderer et al. "*Automatic shortcut removal for self-supervised representation learning*." PMLR, 2020, arXiv:2002.08822)

Martinsite crack



Learn to fill the gap?

Learn placement ?



Potential Avenue: Semi- / Self- Supervised Learning

Possible Avenues:
- X. Zhai, et al. "*S4l: Self-supervised semi-supervised learning*." IEEE/CVF 2019, arXiv: 1905.03670
- J. Grill, et al. "*Bootstrap your own latent: A new approach to self-supervised learning*." arXiv: 2006.07733
- K. Sohn et al. "FixMatch: Simplifying Semi-Supervised Learning [...]" NeurIPS 2020, arxiv: 2001.07685

Variant: Contrastive Learning: Maximize similarity / difference in image pairs
- SimCLR: T. Chen et al. "A Simple Framework for Contrastive Learning of Visual Representations" ICML 2020, arXiv: 2002.05709
- MoCo: K. He et al. "Momentum Contrast for Unsupervised Visual Representation Learning" CVPR 2020, arXiv: 1911.05722
- PIRL: I. Misra et al. "Self-Supervised Learning of Pretext-Invariant Representations" IEEE/CVF 2020, arXiv: 1912.01991
- A. Oord et al. "Representation Learning with Contrastive Predictive Coding" arXiv: 1807.03748

Key Insights:
(A Critical Analysis of Self-Supervision, or what we can learn from a single image, Y. Asano et at., ICLR 2020)

- *"First, we show that as little as a single image is sufficient, when combined with self-supervision and data augmentation, to learn the first few layers of standard deep networks as well as using millions of images and full supervision "*

- Deeper layers: *"For these, self-supervision remains inferior to strong supervision even if millions of images are used for training. Our finding is that this is unlikely to change with the addition of more data."*

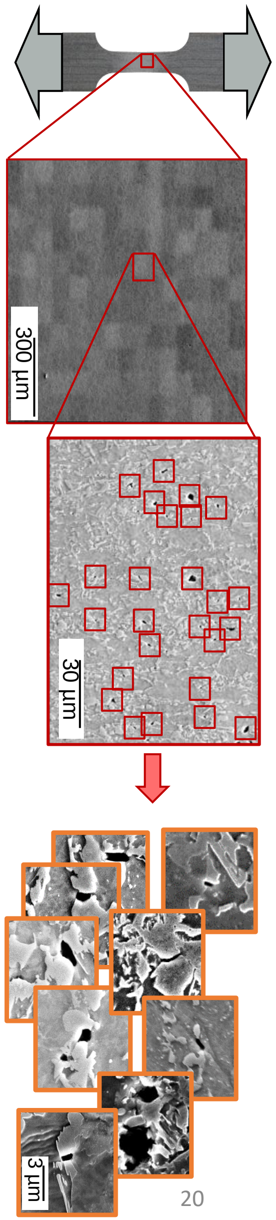
Summary

Deep Learning opens the door to statistical analysis in Materials Science

- Large scale damage identification with high accuracy
- Enables analysis of statistical effects & damage evolution under strain.

<u>Significant challenges remain:</u>
- Damage class definitions – underlying dominant mechanism of damage evolution
- Data handling and metadata
- Supervised learning most accurate and unlikely to be (fully) replacable
  - Large scale image labelling prohibitively costly
  - Many potential avenues to pursue:
    - representation learning + clustering, semi/self-supervised learning, contrastive learning,…
    - As of now: unclear which path most promising for damage analysis

Exciting opportunity for materials science to enter the age of large scale statistical analysis.



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