GO BEYOND

APPLICATION OF MACHINE LEARNING TO MICROSTRUCTURE QUANTIFICATION AND UNDERSTANDING

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OUTLINE

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II. Convolutional neural networks (CNN)
III. Microstructure representations using CNNs
IV. Case Studies:
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   2. Titanium alpha grain segmentation
   3. Titanium cold dwell fatigue prediction
   4. Deep learning model interpretation
V. Conclusion

RECENT PROGRESS IN ARTIFICIAL INTELLIGENCE

The machine learning community has made significant progress in the last 10 years in areas of natural language, computer vision, autonomous decision making, content creation and many others. Many of these technologies naturally extend to materials data.

Speech Recognition

Algorithm Type
Deep Belief Network

Characteristic
Classification

Jan. 2012
Android speech Recognition

Object Recognition

Algorithm Type
Convolutional Neural Network

Characteristic
Make use of local structure.

March 2012
Object Recognition Algorithm Shatters State-of-the-art

Sequential Decision-Making

Algorithm Type
Recurrent Neural Networks

Characteristic
Goal based sequence modeling

May 2015
Algorithms learn to play video games

Jan 2016
AI beats GO champion

Generative Models

Algorithm Type
Generative Adversarial Networks

Characteristic
Learns transferrable visual attributes from images

June 2016
Generative models create realistic images.

How can we leverage these technologies for materials data and engineering?

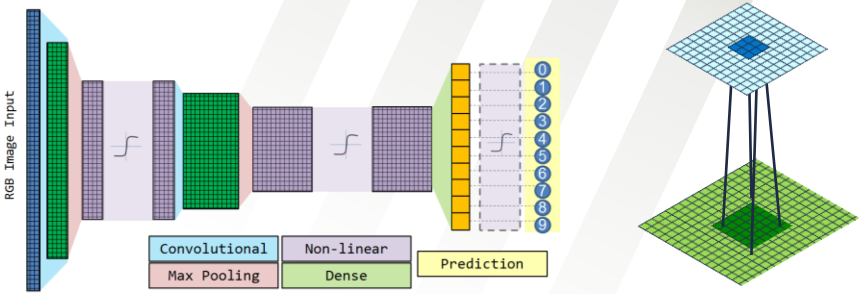
CONVOLUTIONAL NEURAL NETWORKS (CNN)

CNNs are shown to learn low-dimensional spatial statistics that can be used to generate new, statistically equivalent images (bottom right).[1,2]

This information is contained in the various filter activation maps.

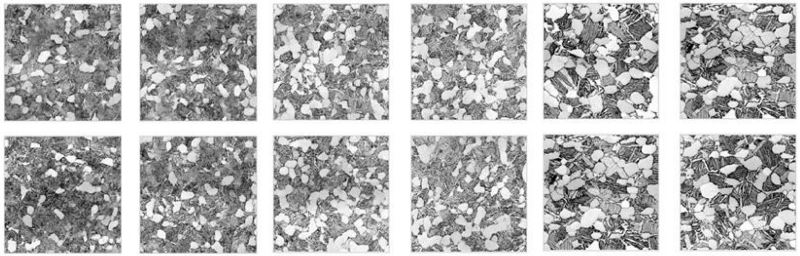
A CNN like VGG16[3] learns over *5000* different filters, has 138,357,544 trainable parameters and was trained on 1.3M images.

Leverage of transfer learning is mandatory when working with smaller datasets.



Source: P&W

Synthetic Microstructure Generation:



Source: P&W

[1] Gatys, L., Ecker, A.S. and Bethge, M., "Texture synthesis using convolutional neural networks. In Advances in Neural Information Processing Systems", 2015
[2] Lubbers, N., Lookman, T., Barros, K., "Inferring low-dimensional microstructure representations using convolutional neural networks", arXiv:1611.02764v1. 2016
[3] Simonyan, K. and Zisserman, A., "Very deep convolutional networks for large-scale image Recognition", arXiv preprint arXiv:1409.1556. 2014.

CNNs learn and apply sequences of stacked convolutional and pooling filters to extract information from images at various length scales that can be used for prediction

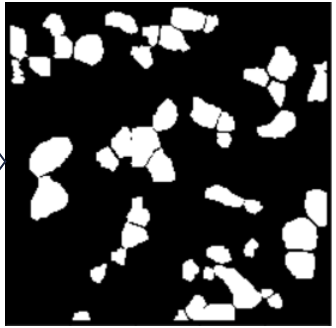
MICROSTRUCTURE REPRESENTATIONS

Microstructure quantification:

- Challenging problem due to microstructure complexity, software, methods, user variability, image quality / mode
- Use of image analysis routines to quantify phase fractions / sizes
- Oversimplified microstructure quantification results in lost information

<u>Standard Microstructure Description</u>

Source: P&W

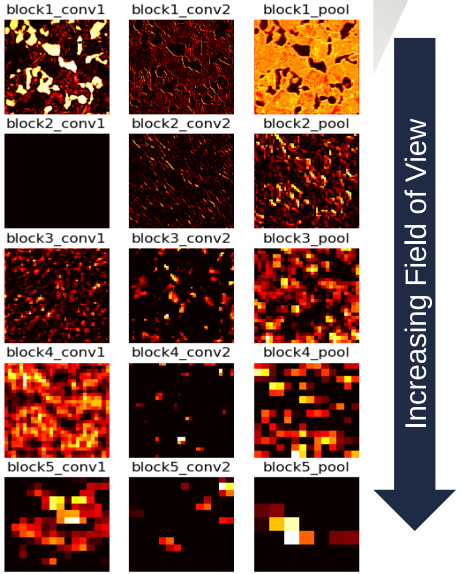


α- fraction

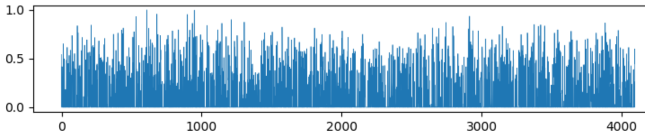
α- grain size

α- lathe thickness

CNN Representations



Spectral output or "fingerprint" for microstructure



Source: P&W

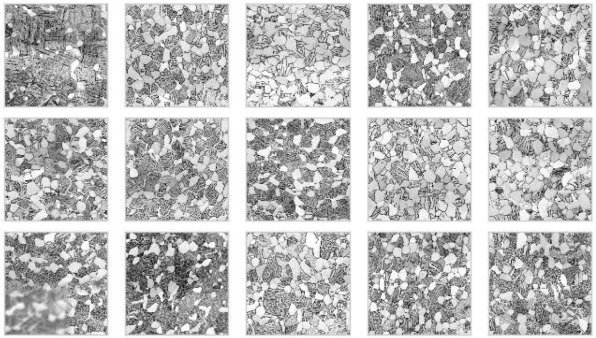
CNNs enable capture of higher-order microstructure statistics and features relative to traditional methods of quantification. This occurs at the expense of interpretability

TI MICROSTRUCTURE CLASSIFICATION FROM DIFFERENT HEAT TREATS

CLASSIFICATION

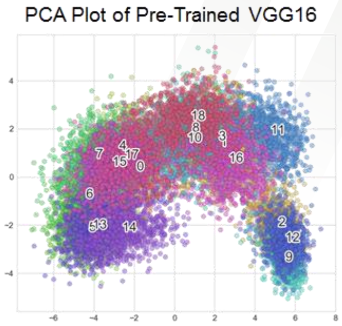
REGRESSION

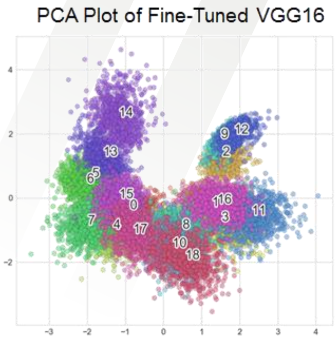
Data:



Source: P&W

Model Results:





Methods:

- ❑ Ti-6Al-4V microstructure dataset was collected
- ❑ 19 different heat treats with varying solution temps, cooling rates, aging times/temps.
- ❑ Over 11,000 images were collected
- ❑ VGG16 final dense layer output run through principal component analysis (PCA)
- ❑ Logistic regression model classification accuracy output recorded vs. number of PCA components

Immediate applications for:

- ✓ Visual similarity assessment / lookup
- ✓ Outlier detection
- ✓ Quality control
- ✓ Process development

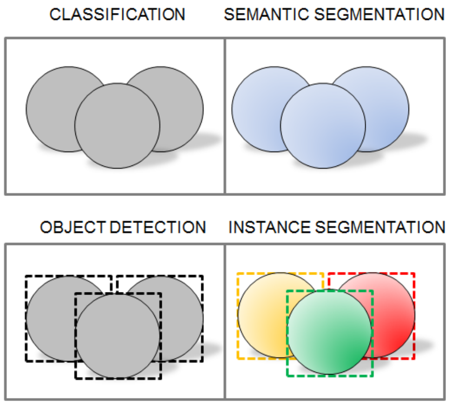
Models are fast -- analyze 100’s of images / second

Pre-trained CNNs are effective for feature extraction. Fine-tuning models for materials microstructure can significantly improve model performance.

MASK RECURRENT-CNN MODELS (RCNN[4]) FOR IMAGE ANALYSIS

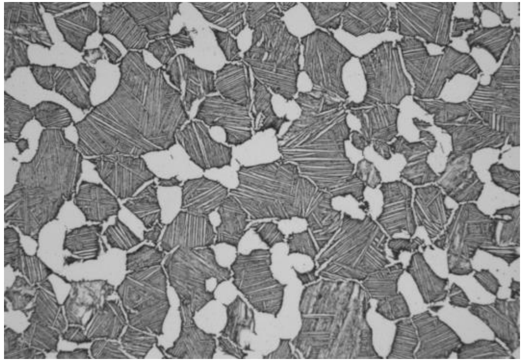
CLASSIFICATION

REGRESSION

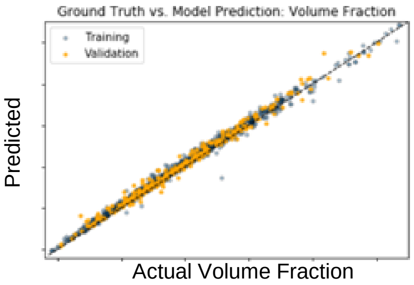


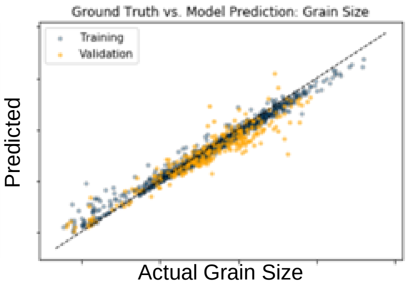
Source: P&W

Input (raw image)



Output (segmented image + stats)





- ❑ Mask-RCNN is able to learn from subject matter experts and significantly reduce turnaround time for microstructure quantification
- ❑ Model is objective and transferrable

[4] He, K., Gkioxari, G., Dollar, P., Girshick, R., Facebook AI Research (FAIR), "Mask R-CNN", arXiv:1703.06870v3 [cs.CV] 24 Jan 2018

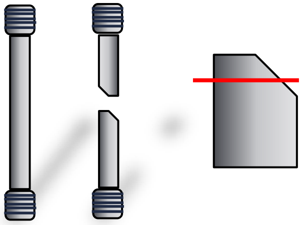
CNNs are powerful and versatile tools for working with image data. There is potential to automate many routine analyses such as phase quantification via image analysis.

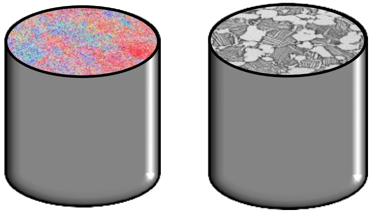
QUANTITATIVE PREDICTIONS USING A CNN: METHODS

CLASSIFICATION

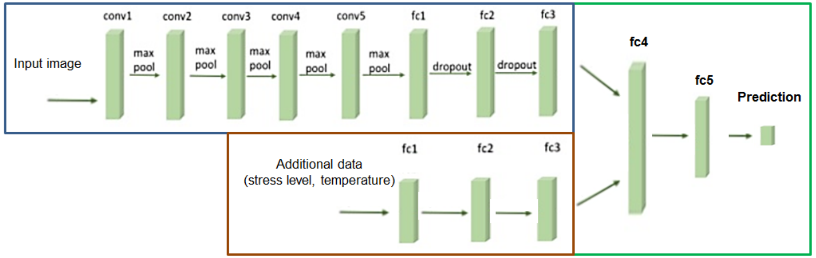
REGRESSION

Mechanical Testing → Characterization:





Modify CNN for Continuous Output:



Learns features from images	Additional data that can't be determined from images	Combines both sources of information to make prediction

Methods:

- ❑ CNNs can make quantitative predictions from images such as strength or fatigue
- ❑ Testing conditions like stress state, temperature, strain rate, specimen geometry, surface treatment cannot be gleaned from images directly, but must be provided to the learning algorithm
- ❑ Relevant test data is concatenated with the output of fully-connected layers
- ❑ Final activation is changed from soft-max to linear. Categorical loss changed to mean squared error

CNNs have demonstrate ability to predict material properties directly from images

QUANTITATIVE PREDICTIONS USING A CNN: CASE STUDY

CLASSIFICATION

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Titanium Dwell Fatigue

- ❑ Dwell fatigue and damage accumulation in Ti64 and Ti6242 is a complex phenomenon involving load shedding between neighboring hard and soft α-hcp grains

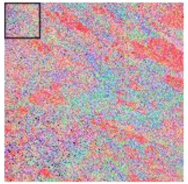
- ❑ Large government, industry and academic collaboration to better understand and predict dwell behavior

- ❑ Electron backscatter diffraction (EBSD) is considered the gold standard for texture description but quantification of critical features and neighborhoods is difficult

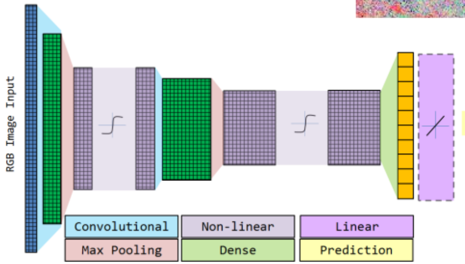
Source: P&W

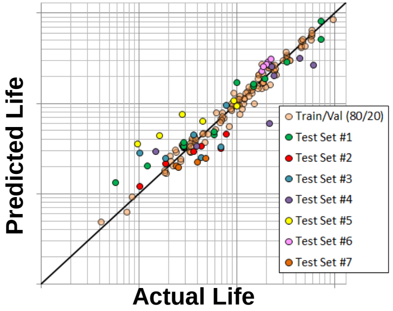
Modeling Approach and Results

- ❑ Use CNN to predict dwell fatigue life using EBSD images from fracture origins of failed specimens (75°F, Kt=1, R=0.05)
- ❑ Test stress, microstructure, and tensile properties were used as supplemental data to the model
- ❑ Sliding window approach used to extract tiles of various sizes from each EBSD image, each of which is assigned the specimen fatigue life



Sliding window crop method





Validated CNN model demonstrates ability to accurately predict specimen-level cold dwell fatigue life from EBSD images –a significant advantage over regression-based methods

BUT WHAT HAS THE MODEL LEARNED?

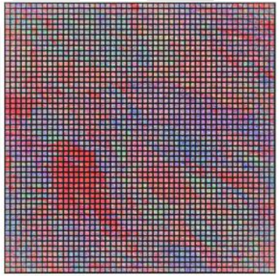
CLASSIFICATION

REGRESSION

Titanium Dwell Fatigue

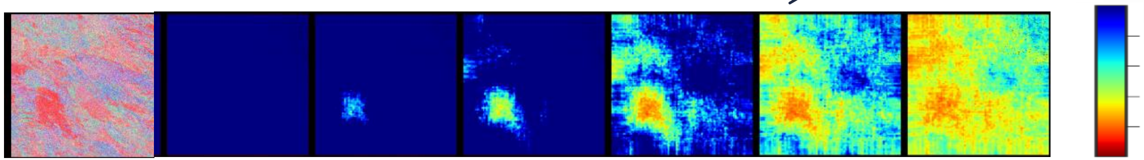
- ❑ Deep learning models are typically considered black boxes
- ❑ CNN regression models can be used to identify critical features and regions within images
- ❑ Enhances model interpretability and user-confidence
- ❑ Models have and continue to be validated on engine hardware and fleet experience

Heavily overlapping sliding windows



EBSD

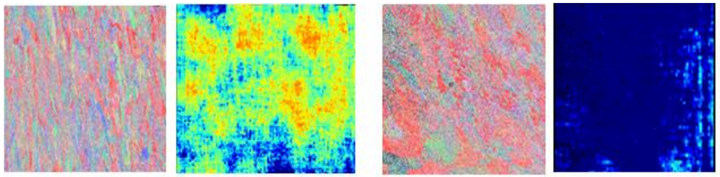
Increasing % of Yield Strength



Product Form Comparison (same test stress)

Billet EBSD

Forging EBSD



Source: P&W

- ✓ CNN can show effect of stress on different microtexture regions
- ✓ CNN can show distinct differences in microtexture activation between different product forms

Investigation of model output shows strong quantitative and qualitative correlation with mechanistic understanding of cold dwell phenomenon

CONCLUSION

Convolutional neural networks can have immediate applications in:

- ❑ Microstructure quality control and anomaly detection
- ❑ Microstructure-sensitive property prediction
- ❑ Image analysis
- ❑ Image similarity assessments

Need to continue working on tools and methods for:

- ❑ Improving model interpretation
- ❑ Incorporating and enforcing mechanistic constraints and prior knowledge
- ❑ Leveraging generative networks to create synthetic materials data for
    - ❑ Microstructure & process optimization
    - ❑ Uncertainty quantification

> Convolutional neural networks are powerful, flexible tools for working with image data

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THANK YOU!

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