Automated recognition and quantification of dual phase titanium alloy microstructures using convolutional neural networks

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ABSTRACT

Recent advances in machine learning and image recognition tools/methods have been used to address fundamental challenges in materials engineering e.g. the automated classification and quantification of microstructure images. In this work, a total of 19 different Ti-6Al-4V microstructures were produced by varying heat treat parameters such as solution temperature, cooling rate, aging times and temperatures. Over 14,000+ microstructure images were collected and able to be classified by heat treat ID with greater than 90% validation accuracy using the outputs of a pre-trained convolutional neural network (CNN) and a logistic regression model. These image classification models were then used to determine and justify statistically equivalent representative volume elements (SERVE). Lastly, a convolutional neural network was trained and validated to make accurate quantitative predictions for primary alpha volume fraction from synthetic and real, two-phase image datasets.

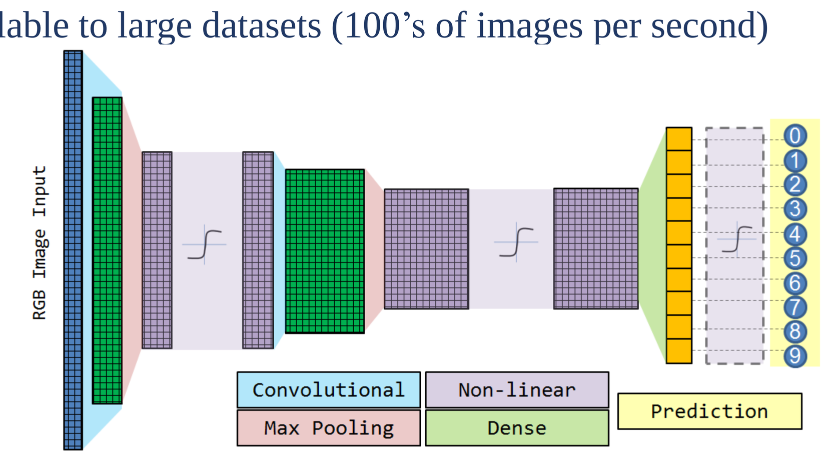
BACKGROUND

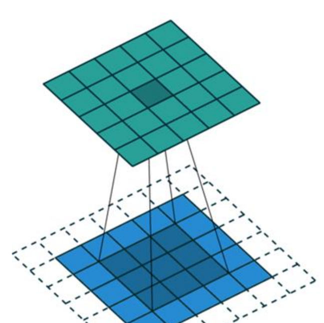
Conventional Microstructure Analysis:

- Largely reliant on domain expertise, institutional knowledge, and visual conformity to established materials specifications.
- Calculation of grain sizes and phase fractions require the use of image analysis software
- Repeatability and reproducibility difficult due to variation in sample prep, imaging, software
- Current methods are not scalable to large datasets

Convolutional neural networks (CNNs):

- Widespread adoption in the image domain
- Have enabled great strides in object detection, image classification and image segmentation
- Automatically learn spatial information and critical features at various length scales
- Scalable to large datasets (100's of images per second)

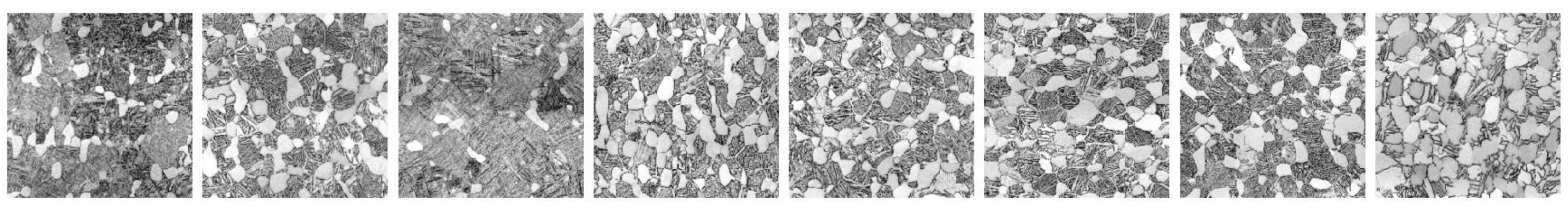




DATA AND METHODS

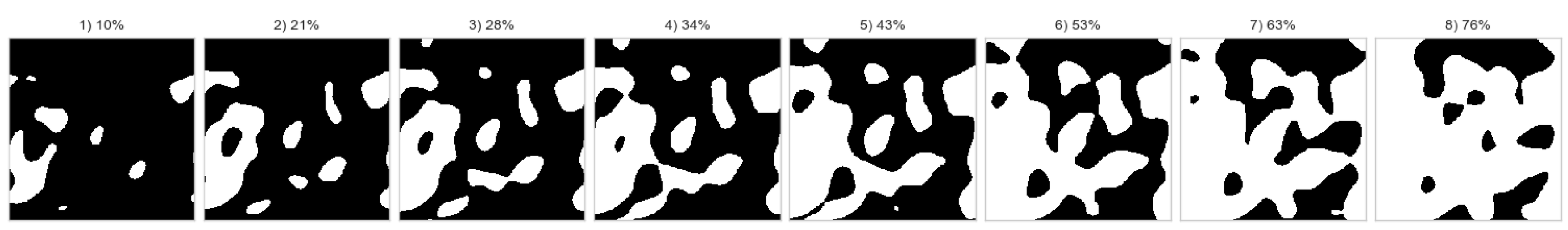
1) Microstructure Classification Dataset:

- Size: 14,000 images (Ti-6Al-4V)
- Pedigree: 19 different heat treatments (varying solution temperature & cooling rates) – equal class balance
- Problem statement: Can a CNN match microstructure images to the corresponding heat treatment?
- Modeling approach:
    - Image feature extraction using pre-trained VGG16, followed by dimensionality reduction and training of logistic regression model.
    - Fine-tune VGG16 on microstructure images and predict heat treat ID directly
    - Data was split 80/20 for training and validation. Real time data augmentation to reduce overfitting.



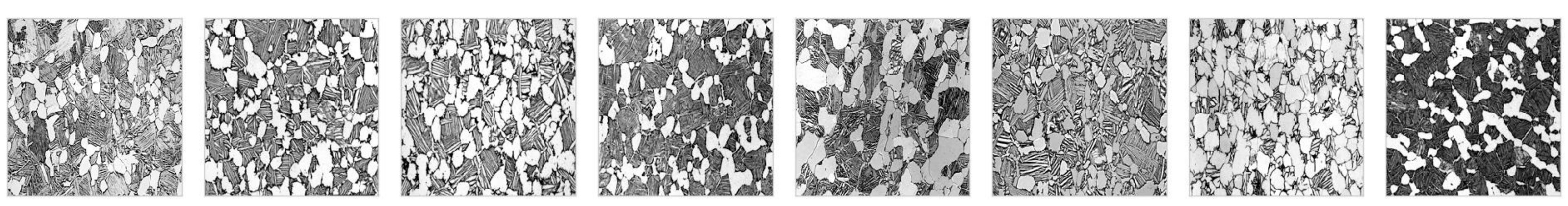
2) Synthetic Two-Phase Dataset:

- Size: 5,000 images (binary)
- Pedigree: White phase fraction ranging from 10-80%
- Problem statement: Can a CNN quantitatively predict phase fraction of white pixels in images?
- Modeling approach:
    - Modify VGG16 model by replacing soft-max classification layer with a dense layer of unit size to enable prediction of a single per training image. Also swap default 'categorical_crossentropy' loss function for 'mean_squared_error'
    - Data was split 80/20 for training and validation. Real-time data augmentation used to reduce overfitting.



3) Alpha-beta Microstructures ("in the wild") Dataset:

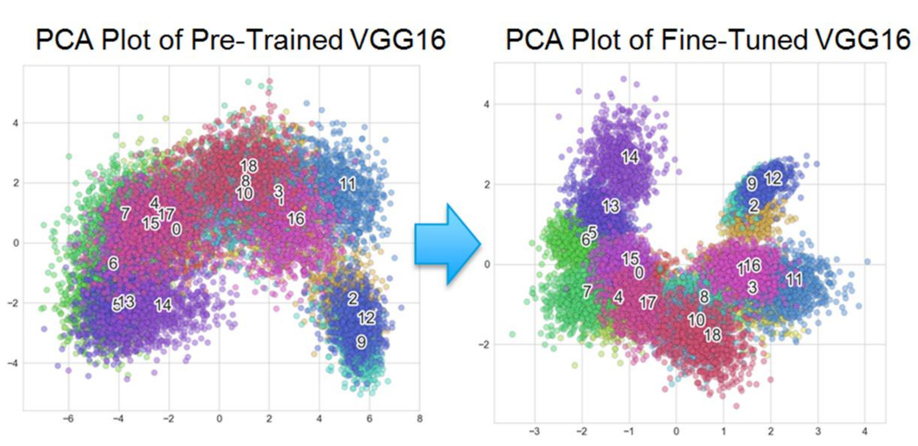
- Size: 2190 images (Ti-6Al-4V, Ti-6Al-2Sn-4Zr-2Mo)
- Pedigree: Various billet, bar, forging microstructures (with natural variability in image quality)
- Problem statement: Can a CNN predict primary alpha volume fraction directly from images?
- Modeling approach:
    - Same model that was used from Dataset #2 (see above).

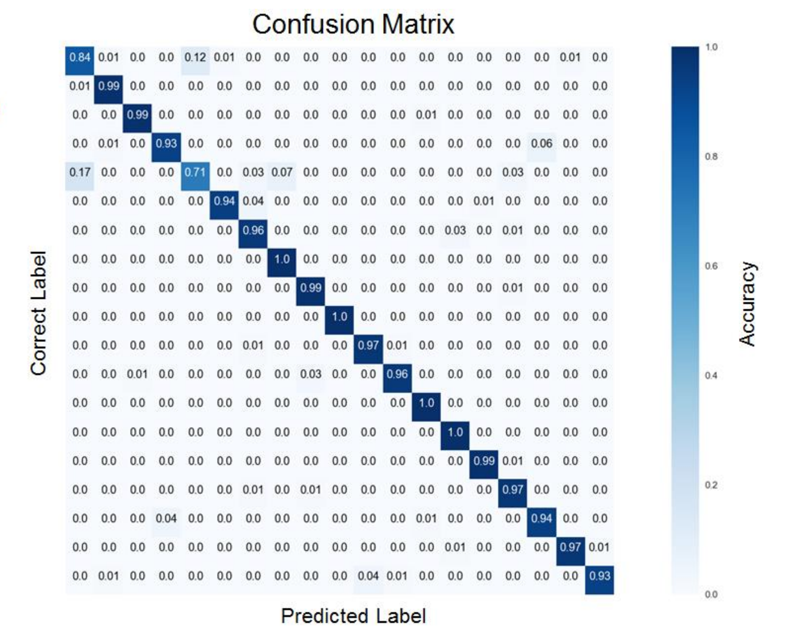


RESULTS

Microstructure Classification:

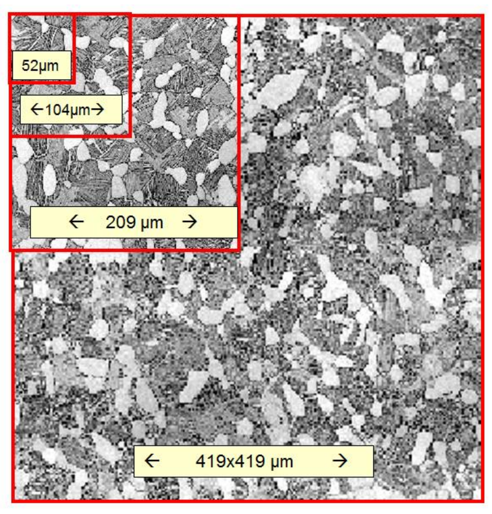
Image feature vectors (4096 dimensional) were obtained after running images through the pre-trained VGG16 model. Principal component analysis (PCA) was used to reduce dimensionality for visualization and prior to fitting a logistic regression model for image classification. The classifier achieved a k-fold cross validation (k=10) accuracy of 83% using 20 PCA components. A scatterplot of the first two PCA components is shown below, where point colors indicate class label. Clustering of points is observed and the distance between points can be used as an indicator of visual similarity. After fine-tuning the VGG16 model, cluster definition was enhanced which is in agreement with the improved accuracy (95%) on the validation dataset of 2800 images. A confusion matrix is provided to show classification accuracy for each of the 19 alloy pedigrees and where misclassifications occurred.

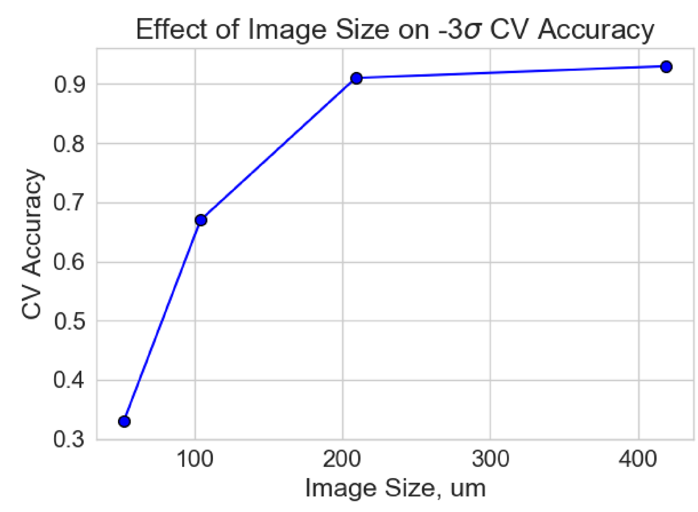




Microstructure SERVE assessment:

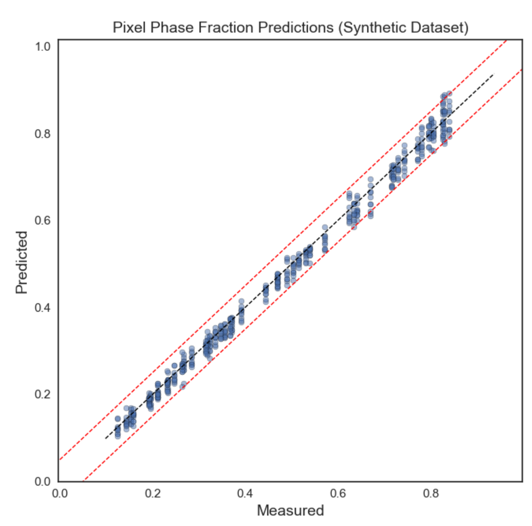
In many applications, it is important to be able to identify the statistically equivalent representative volume element (SERVE), which is the minimum area/volume needed to statistically describe a microstructure. Using the logistic regression model performance as the baseline, logistic regression model cross-validation accuracies are compared as a function of input image size. It was found that small image sizes (52um x 52um), cross-validation accuracies were less than 40%. For 104um x 104um images, the accuracy increases to approximately 70%. At 209um and 419um images, the accuracy plateaus around 91-93%, respectively. This exercise suggests that the SERVE for this titanium dataset is approximately 209um x 209 um, below which the classifier is unable to reliably separate the various microstructures.

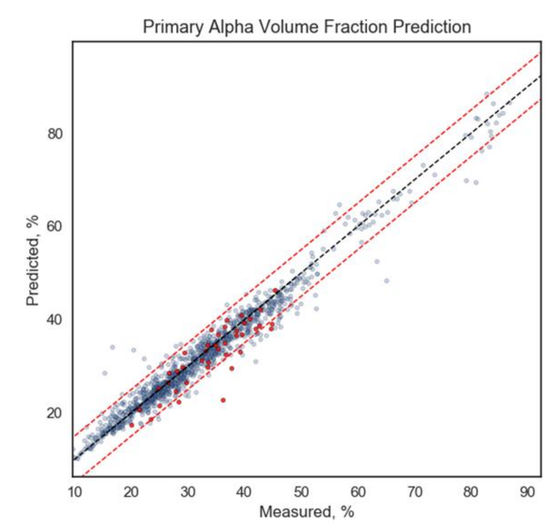




Microstructure Quantification:

All the prior work has focused on classification of microstructure images. A natural extension of this work is to infer continuous value properties from image directly e.g. material properties or processing routes –without explicitly quantifying features and building response models. Below (left) shows predictions of pixel phase fraction for the synthetic validation dataset (500 images) –demonstrating good performance on new data. Below (right) shows the performance of a CNN in predicting primary alpha volume fraction for the training set and a separate validation set (in red). The positive results indicate that CNN models are able to accurately predict phase fractions from images directly, bypassing the need for traditional image analysis. The model successfully overcomes natural and artificial variation in image quality as it learns to identify primary alpha grains –not from an absolute RGB pixel value but from other visual characteristics used by skilled practitioners.





REFERENCES

[1] Fullwood, W., Niezgoda, S., Kalidindi, S., "Microstructure reconstructions from 2-point statistics using phase-recovery algorithms", Acta Materialia 56(5):942:948, 2008.

[2] Simonyan, K. and Zisserman, A., "Very deep convolutional networks for large-scale image Recognition", arXiv preprint arXiv:1409.1556. 2014.

[3] Gatys, L., Ecker, A.S. and Bethge, M., "Texture synthesis using convolutional neural networks. In Advances in Neural Information Processing Systems", (pp. 262-270). 2015

[4] Lubbers, N., Lookman, T., Barros, K., "Inferring low-dimensional microstructure representations using convolutional neural networks", arXiv:1611.02764v1. 2016

[5] Larsen, A.B.L, Sonderby, S, Larochelle, H. and Winther, O., "Autoencoding beyond pixels using a learned similarity metric", arXiv:1512.09300v2 [cs.LG] 10 Feb 2016

[6] LeCun Y, Bengio Y., "Convolutional networks for images, speech, and time series", The Handbook of Brain Theory and Neural Networks. Apr; 3361(10):1995.

[7] Erhan, D., Courville, A., and Bengio, Y., "Understanding representations learned in deep architectures. Department d'Informatique et Recherche Operationnelle, University of Montreal, QC, Canada, Tech. Rep, 2010.

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