Feedstock optimization using computer vision and machine learning techniques

CASIS Workshop

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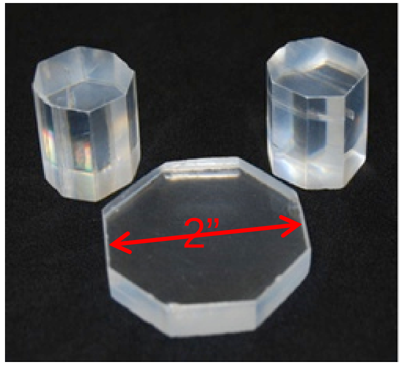
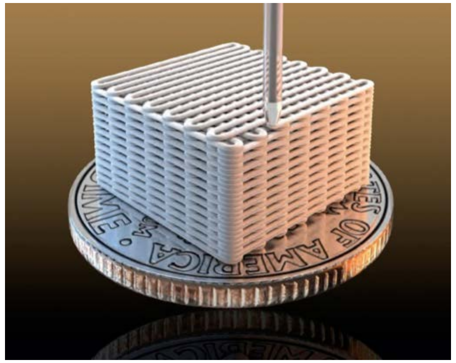
Success of LLNL and our partners' missions requires timely development and deployment of diverse materials



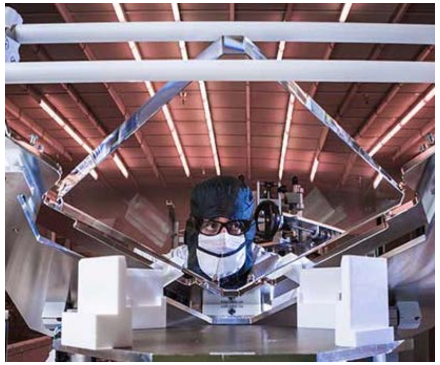
Plastic scintillators

Energetic Materials

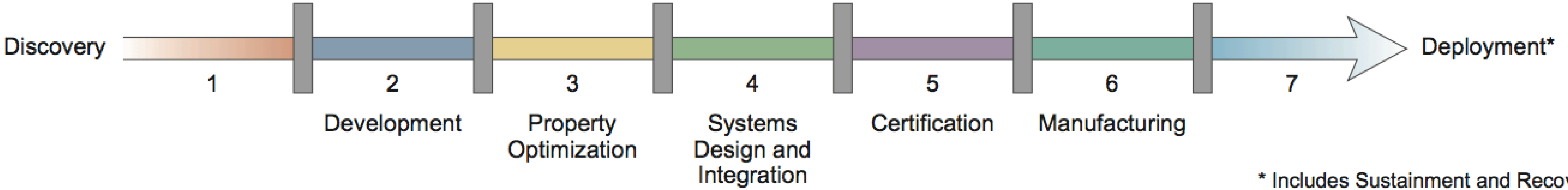
Porous Materials



AM components



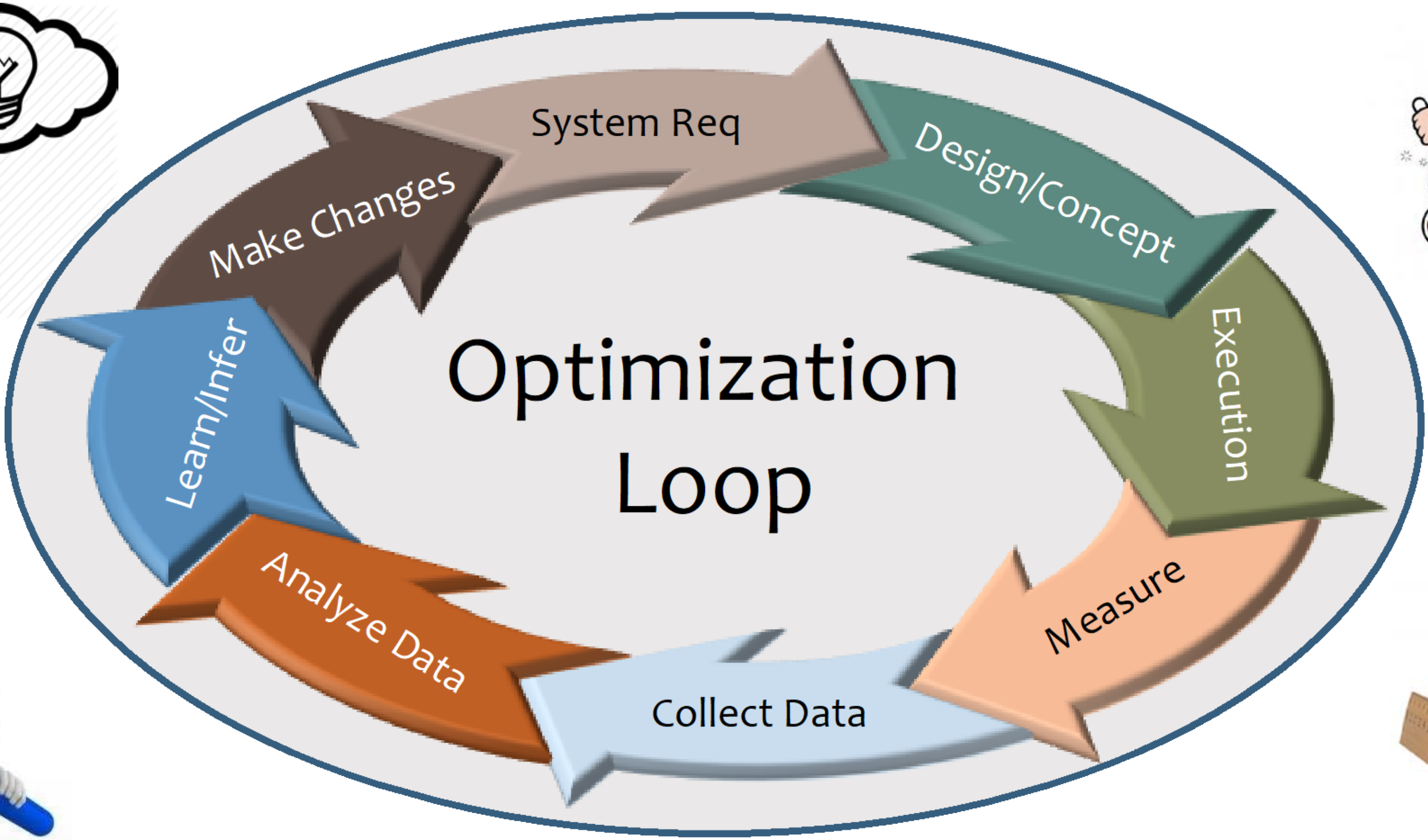
Optical Materials



* Includes Sustainment and Recovery

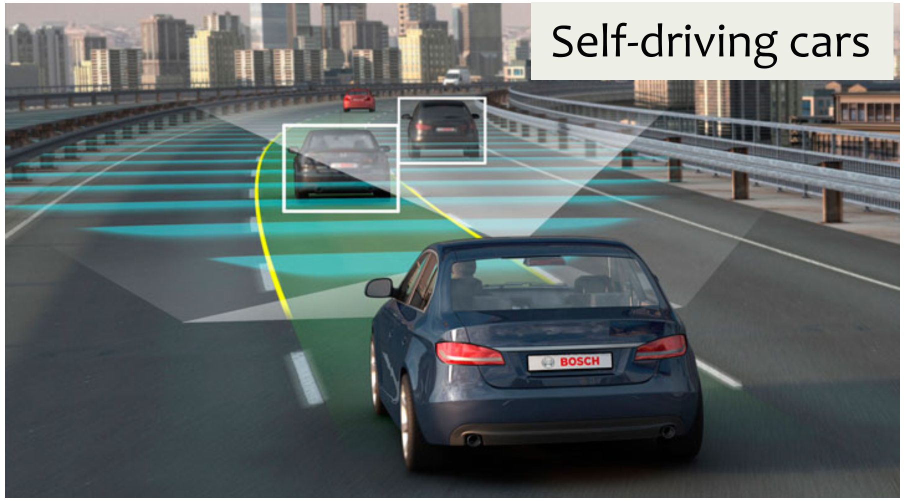
Our group focuses on accelerating materials development, optimization and deployment, while providing performance and compatibility predictions during the lifetime of the materials

Materials discovery, development and deployment requires many iterations

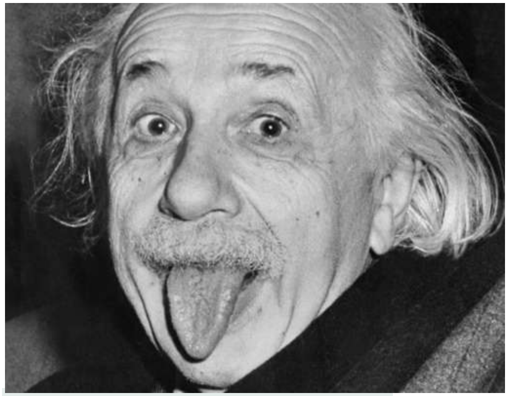


Success with less Iteration

Artificial Intelligence has made tremendous progress in recent years

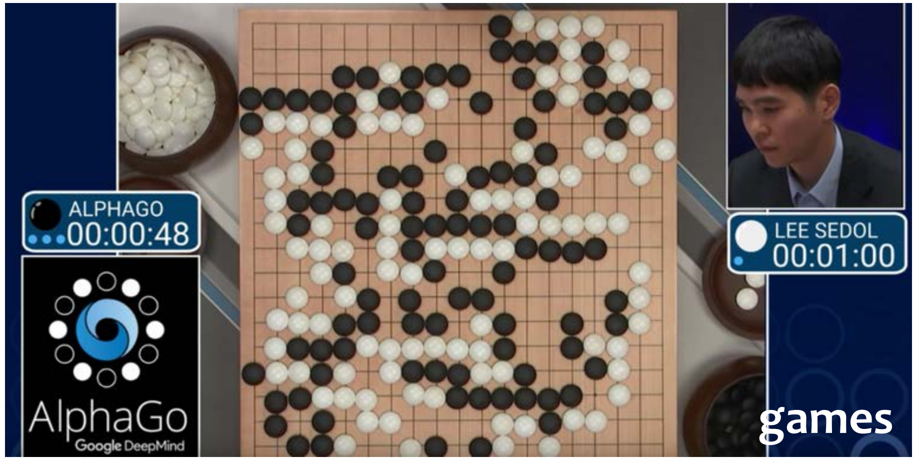


Self-driving cars



Face Recognition

Smart Home

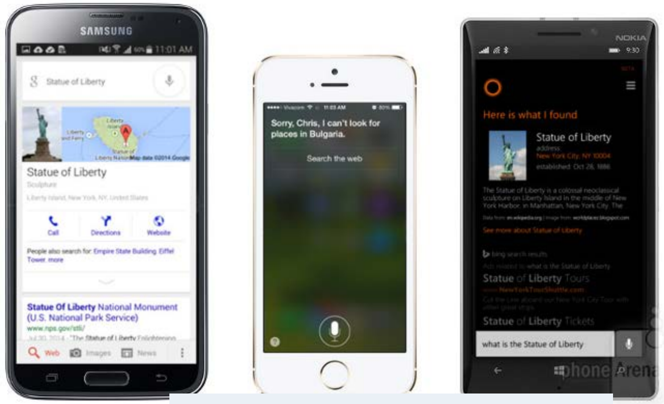


games

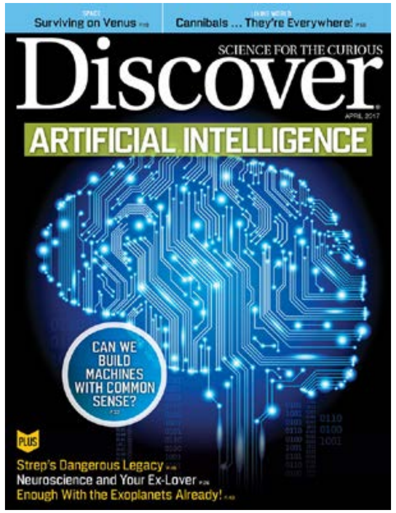
Google Now

Siri

Cortana



Personal Assistants



Application of ML to materials science requires overcoming many challenges

Materials Science Challenges

- Materials Discovery
- Synthesis & Performance Prediction
- Rapid Materials Attribute Characterization and Analysis
- Materials Process, Property, Performance Correlation
- Aging and Lifetime Prediction
- Certification & Qualification

Implementation of Existing Tools

Optimization of existing tools

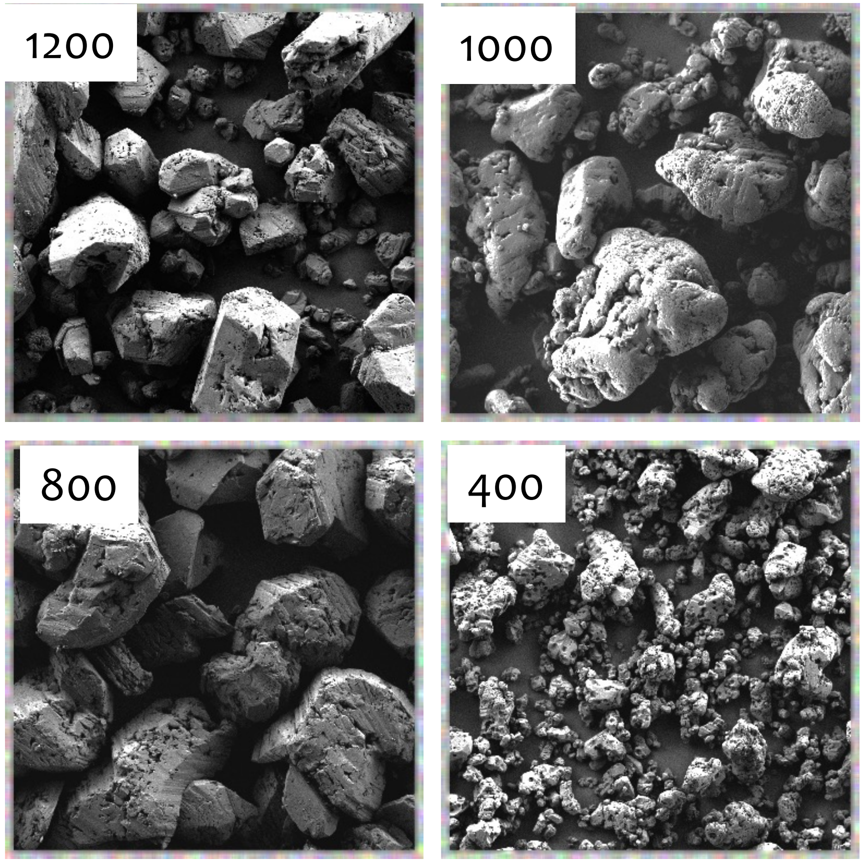
New tool development

M.L. and Data Science Challenges

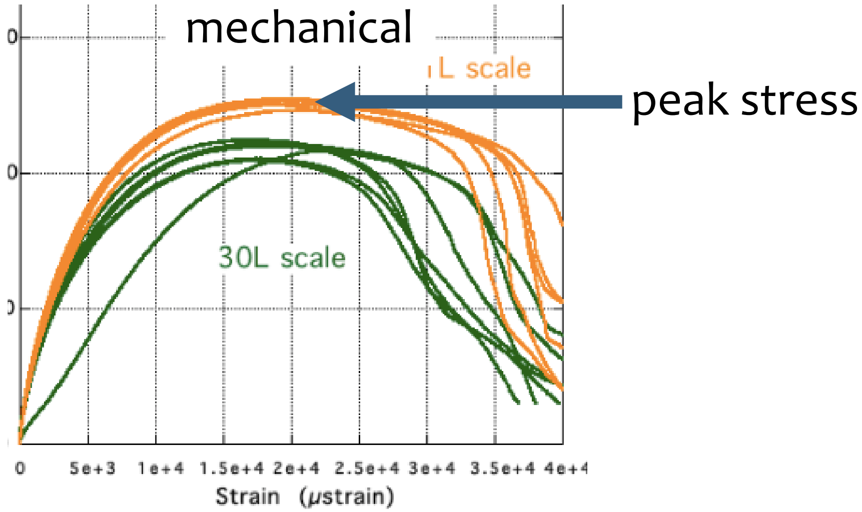
- Explainability
- Feature Engineering
- Small Data
- Confidence Level
- Generalizable ML
- Multiple Data Source
- Domain Knowledge Incorporation

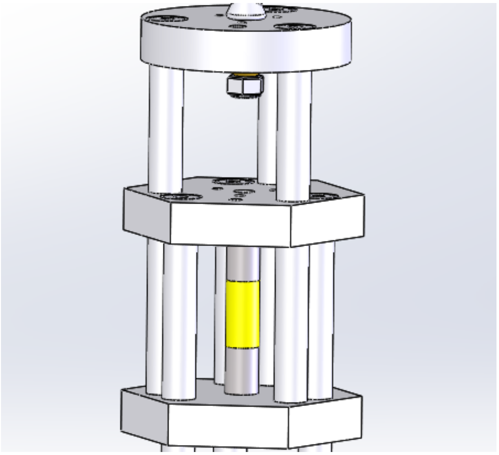
There are preliminary results to show ML can help Materials Science

Material attributes dictate performance



impacts

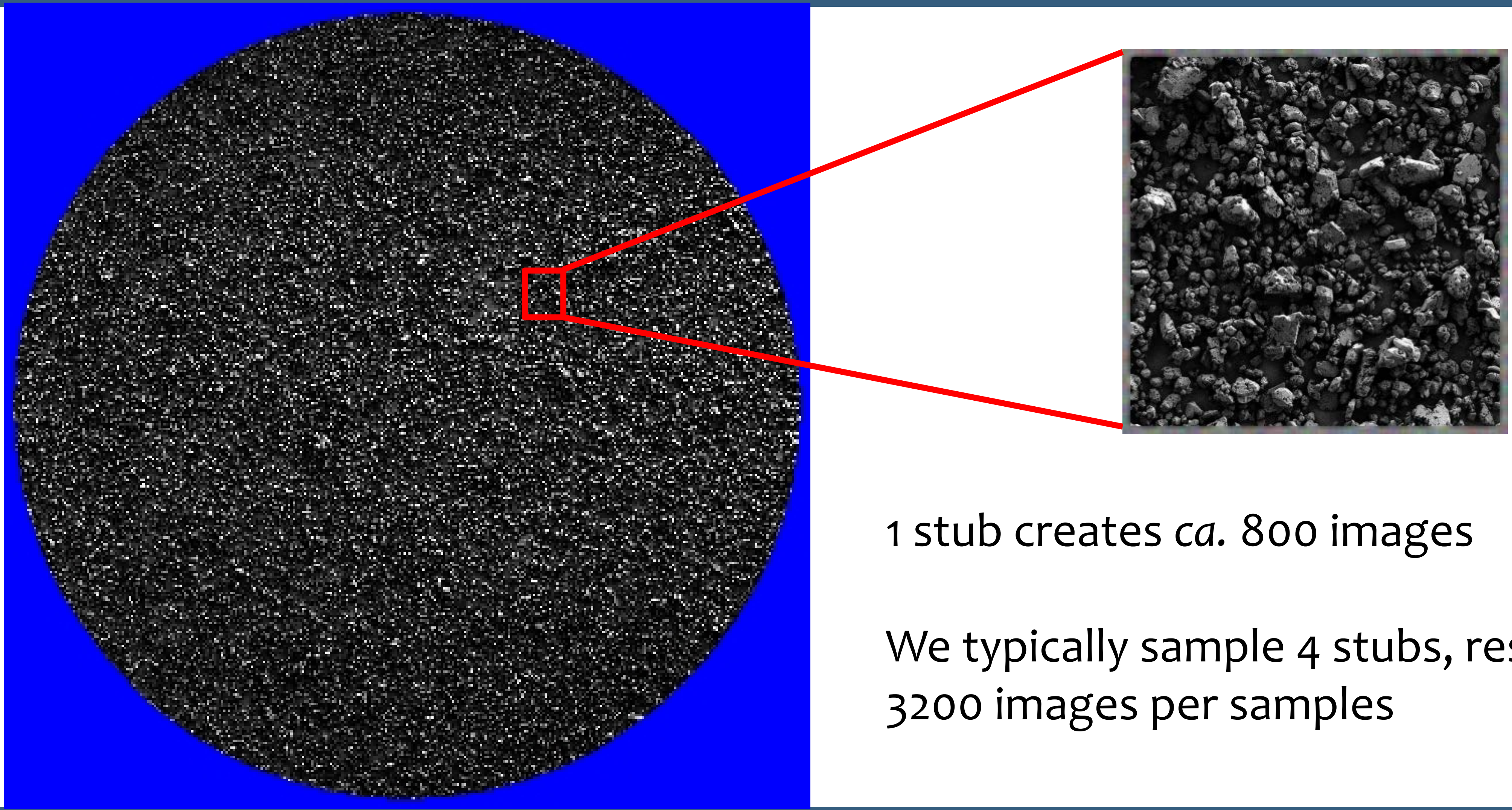




compression testing

Materials attributes: particle size, morphology, surface area, voids, surface texture, aggregation, density, etc.

Automated image collection with Zeiss SEM allows for rapid collection of thousands of images

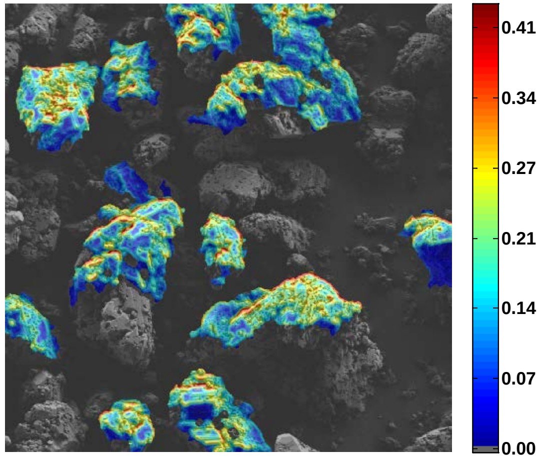


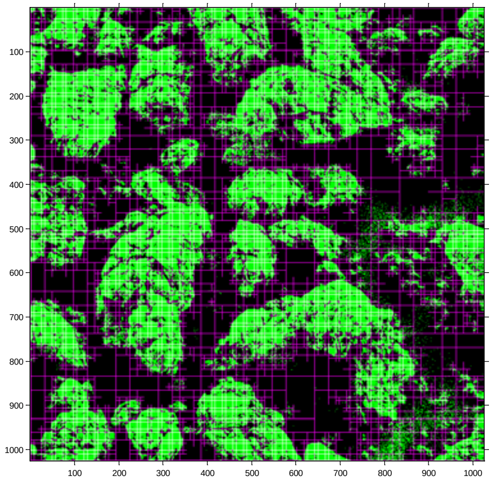
1 stub creates *ca.* 800 images

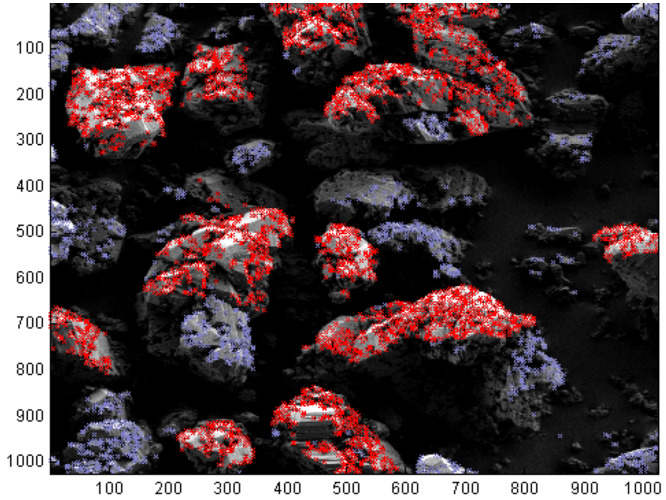
We typically sample 4 stubs, resulting in 3200 images per samples

We are using computer vision tools/ML and Deep Neural Network approaches to study SEM images

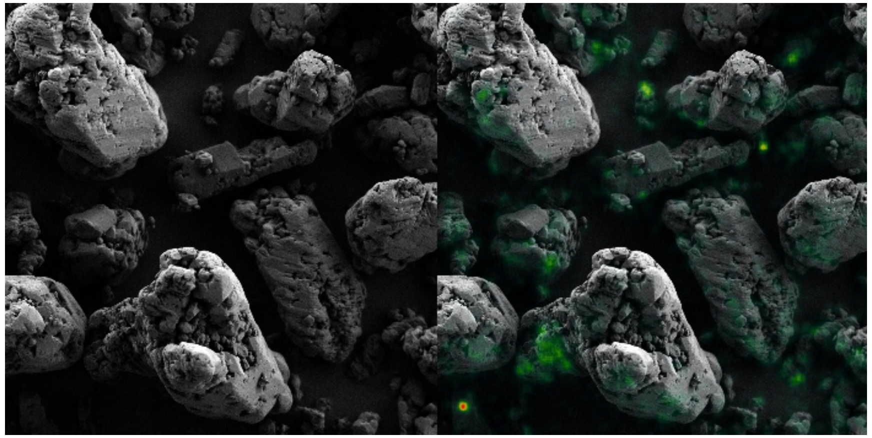
Traditional Approach:
Computer Vision/ML

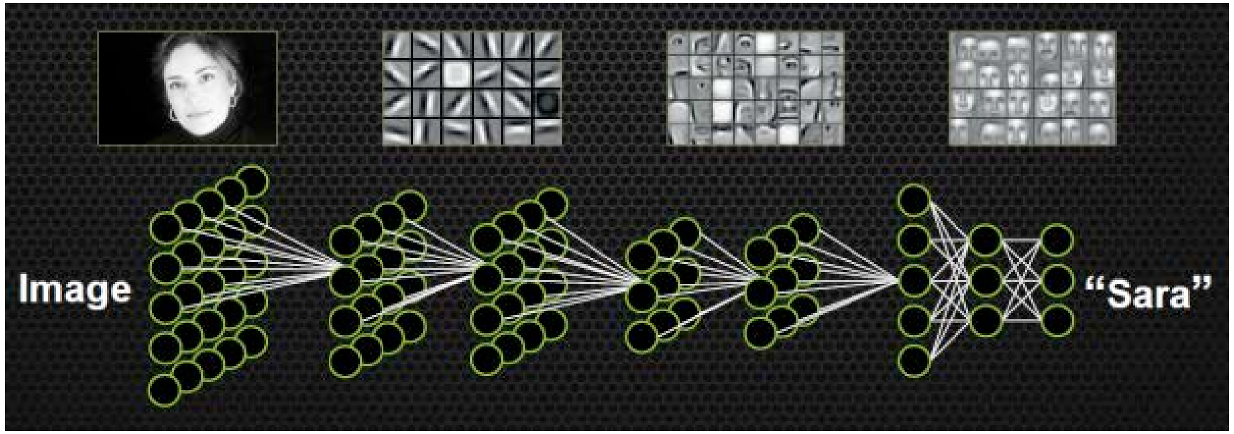




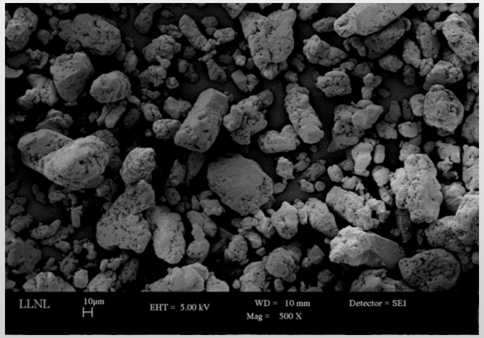


Deep Neural Network Approaches:



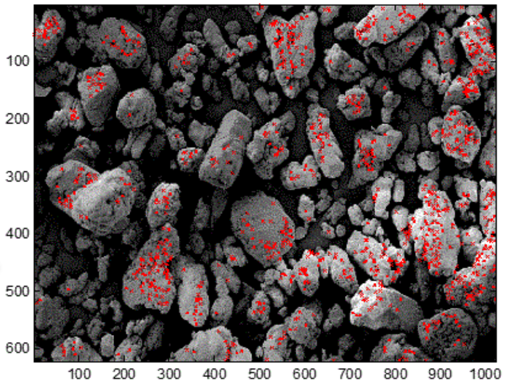


CV tools can extract quantifiable feature values and ML models can be used to correlate to performance

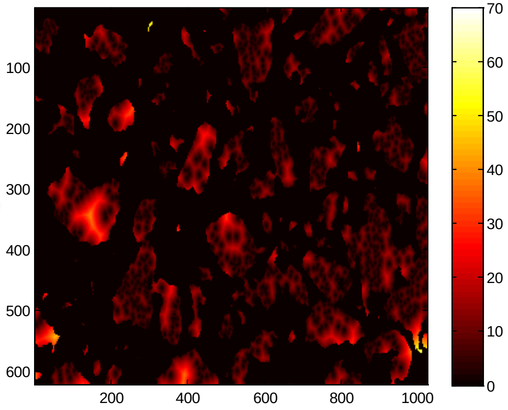


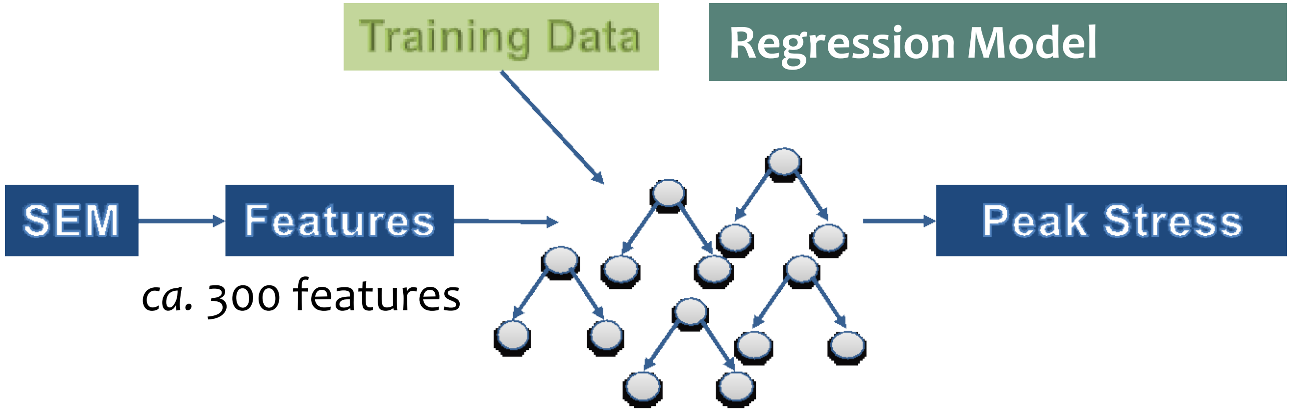
Original SEM Image

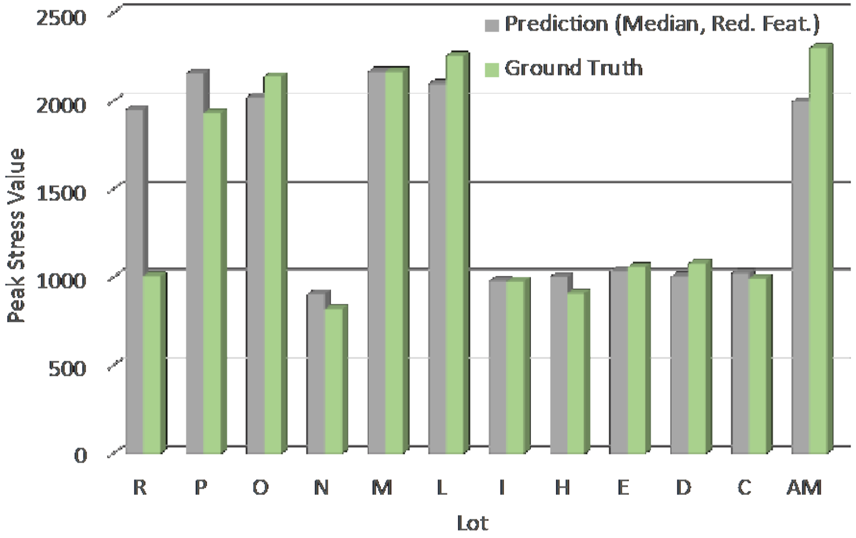
Corner Detection



Corner Distance Metric







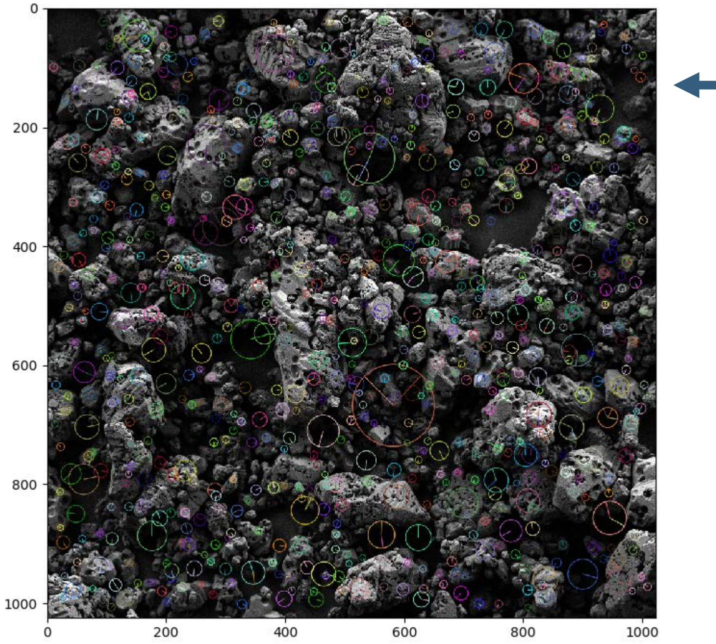
Data Source

80k SEM images
Labeled with peak stress data

Bag of Visual Words Approach

Bag-of-visual-words approach:

-Compute well known features + descriptors (e.g. scale-invariant feature transform (SIFT))
-Cluster descriptors into k bins (k-means clustering)
-The histogram of these bins (the bag-of-visual words) now describes the image and can be used for classification or regression
-This technique has been successfully used to classify materials from images [1,2,3]



SIFT key-points detected on SEM image

1. DeCost, B. L.; Holm, E. A., Characterizing powder materials using keypoint-based computer vision methods. Comput. Mater. Sci. 2017, 126, 438-445.
2. Chowdhury, A.; Kautz, E.; Yener, B.; Lewis, D., Image driven machine learning methods for microstructure recognition. Comput. Mater. Sci. 2016, 123, 176-187.
3. DeCost, B. L.; Holm, E. A., A computer vision approach for automated analysis and classification of microstructural image data. Comput. Mater. Sci. 2015, 110, 126-133

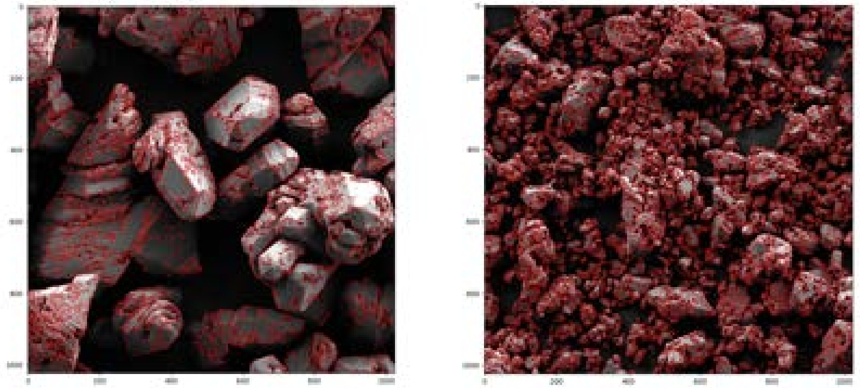
SEM image features- Domain knowledge incorporated

Try features that specifically relate to particle sizes and textures:

- Canny edge detection (count “on” edge pixels)
- Fourier/frequency analysis
- **Binarized Statistical Image Features (BSIF)[4]**

Implemented in Python

Canny edge detection



Low peak-stress sample   High peak-stress sample

BSIF

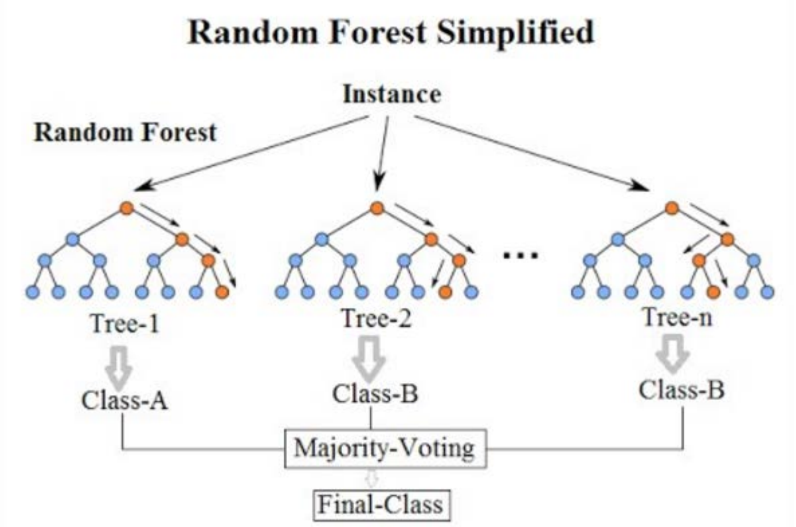
Samples from CUReT database (top) and corresponding BSIF codes.

4. Kannala J & Rahtu E: "BSIF: binarized statistical image features", ICPR 2012.

Material performance regression

- Numerous performance metrics are available. We chose peak-stress of the stress-strain curve as our "label".

- Many regression models can be used:
  - Linear
    Support Vector
    Gradient Boosting
    Random Forest
    others

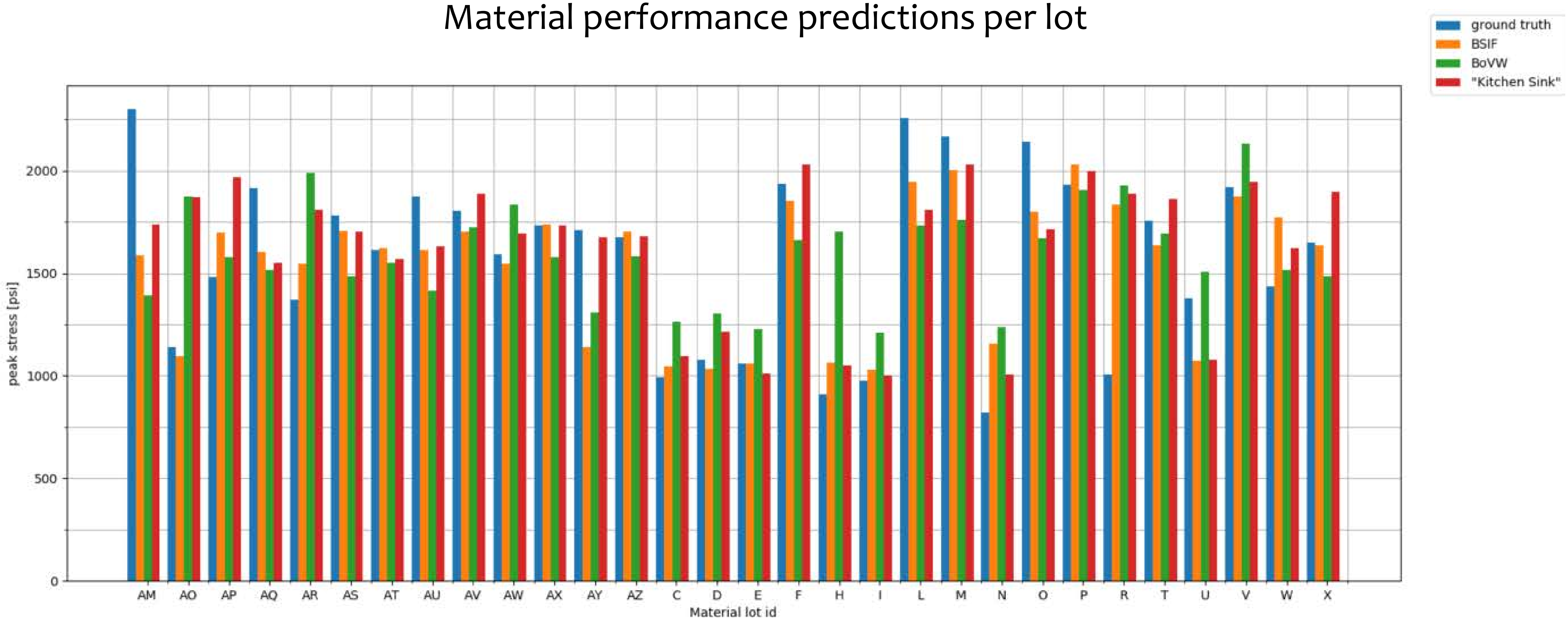


- We chose random forest due to its versatility, its ability to provide accuracy without tuning meta-parameters, and its ability to provide feature importance once trained

- Cross-validation performed with leave-one-out protocol—For each lot, train on everything else but that lot, then predict performance for that lot

Material performance regression

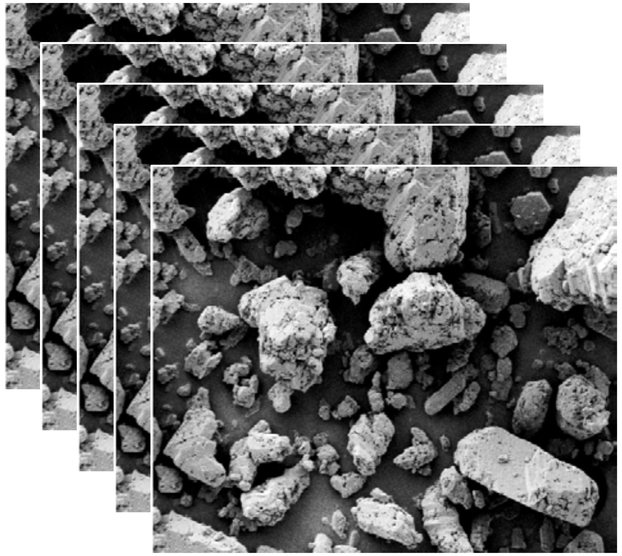
Material performance predictions per lot

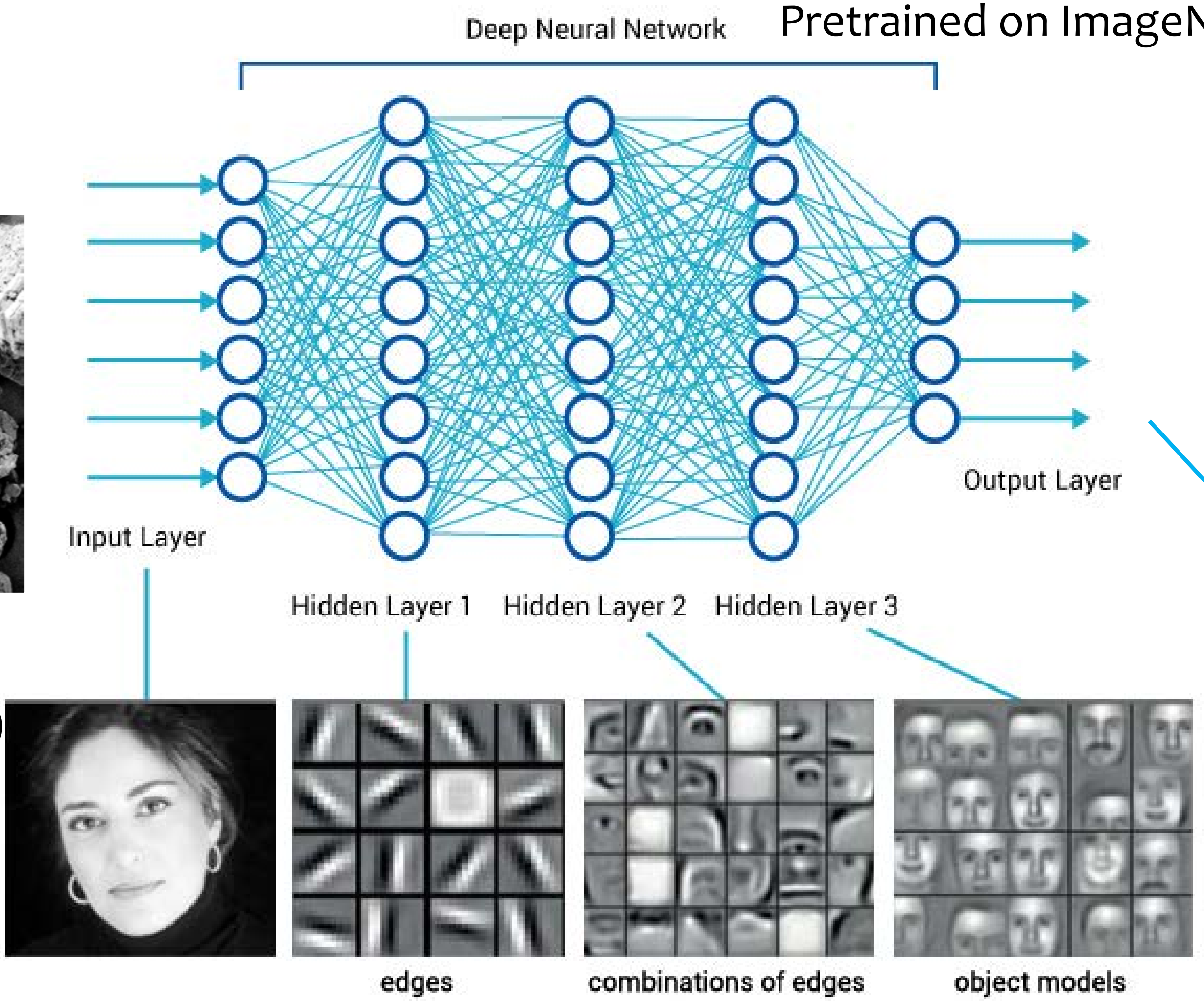


Overall, BSIF had the best performance as measured by RMSE. (BSIF: 252 psi, BoVW: 390, KS: 280)

Deep learning for SEM/image analysis

70k images (20+ lots)





Pretrained on ImageNet

1. DenseNet (CNN)
2. Inception (CNN)

Compression Peak Stress = 1500 psi

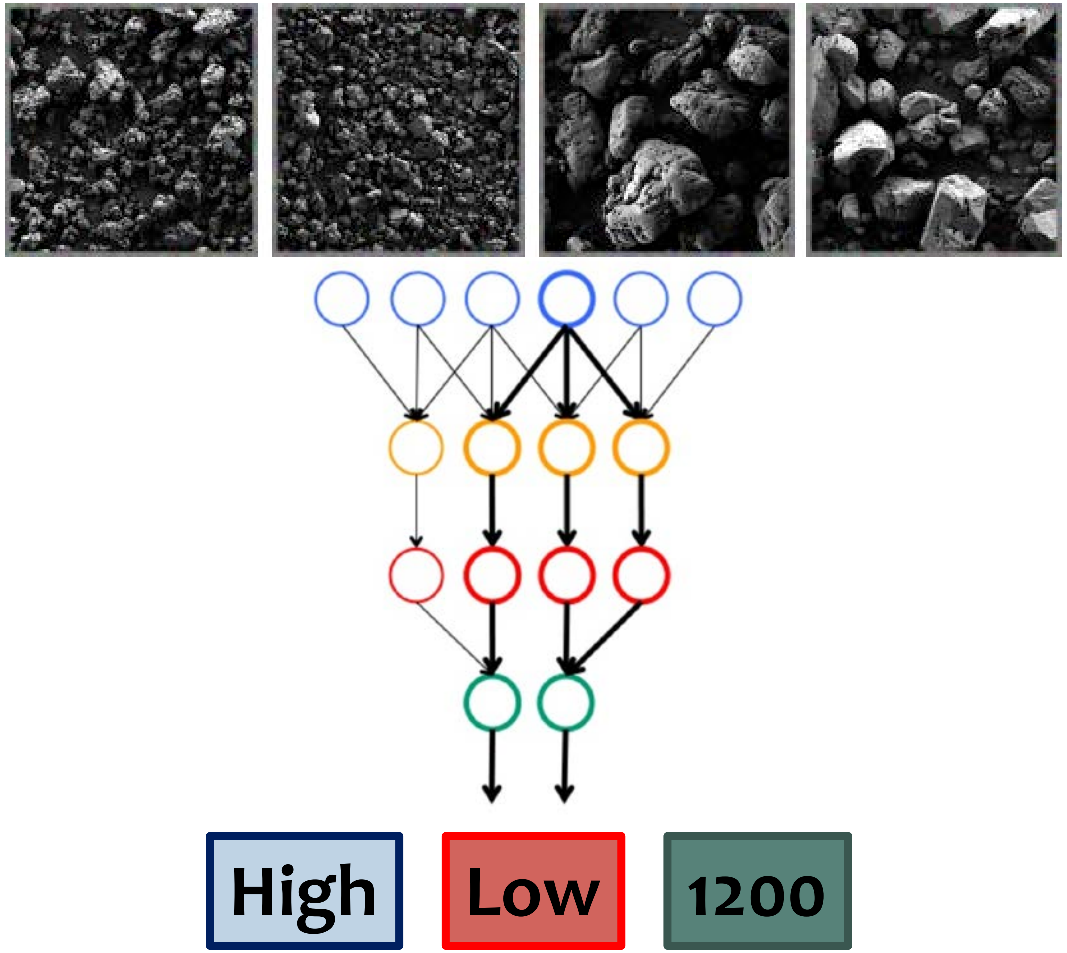
SARA

Other examples of inputs

- CT (25 samples, 145K images)
- Surface area
- Particle size analysis
- density
- Etc.

Training and Methodology

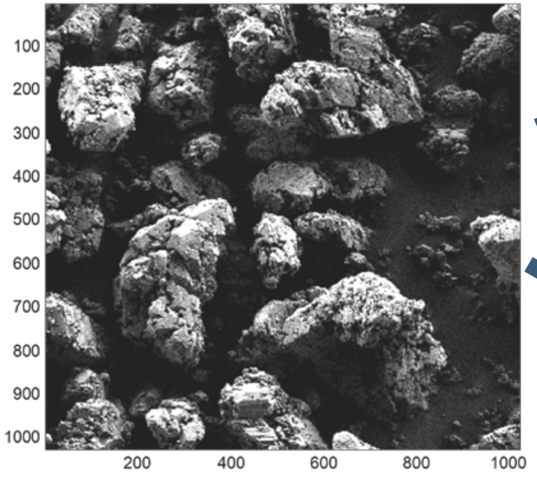
- We train a deep learning network (Dense Net) to give the estimated corrected peak stress (PS) for a patch.
  - The input is a single SEM patch from Atlas.
  - The output is an estimated regression value (peak stress) or classification classes (high or low).
- We use a leave-one-out cross validation where a single batch is left out and used for validation. We do this n times for each batch.
  - This allows us to estimate performance for unseen novel batches.
- We combine the scores over all patches to create an estimated PS per batch.
- We tried some variations on input images to try and improve performance.



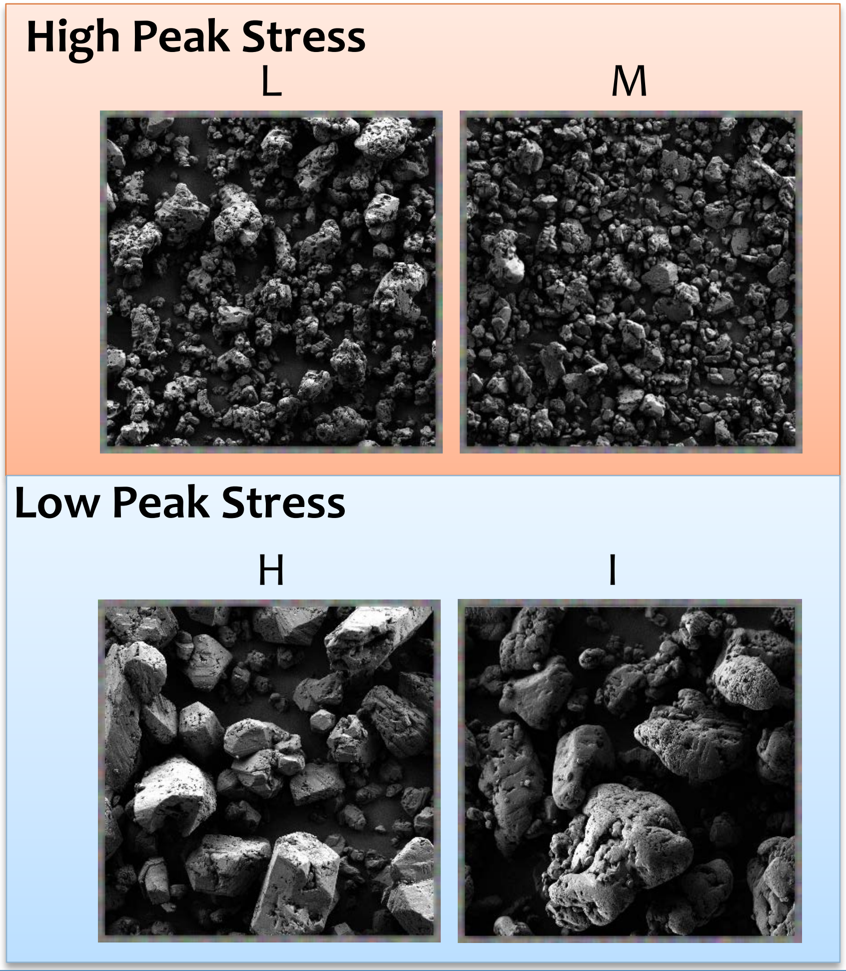
DNN can be used to create empirical models to predict performances

classification

New lot



?



Examine Further

Get to it later

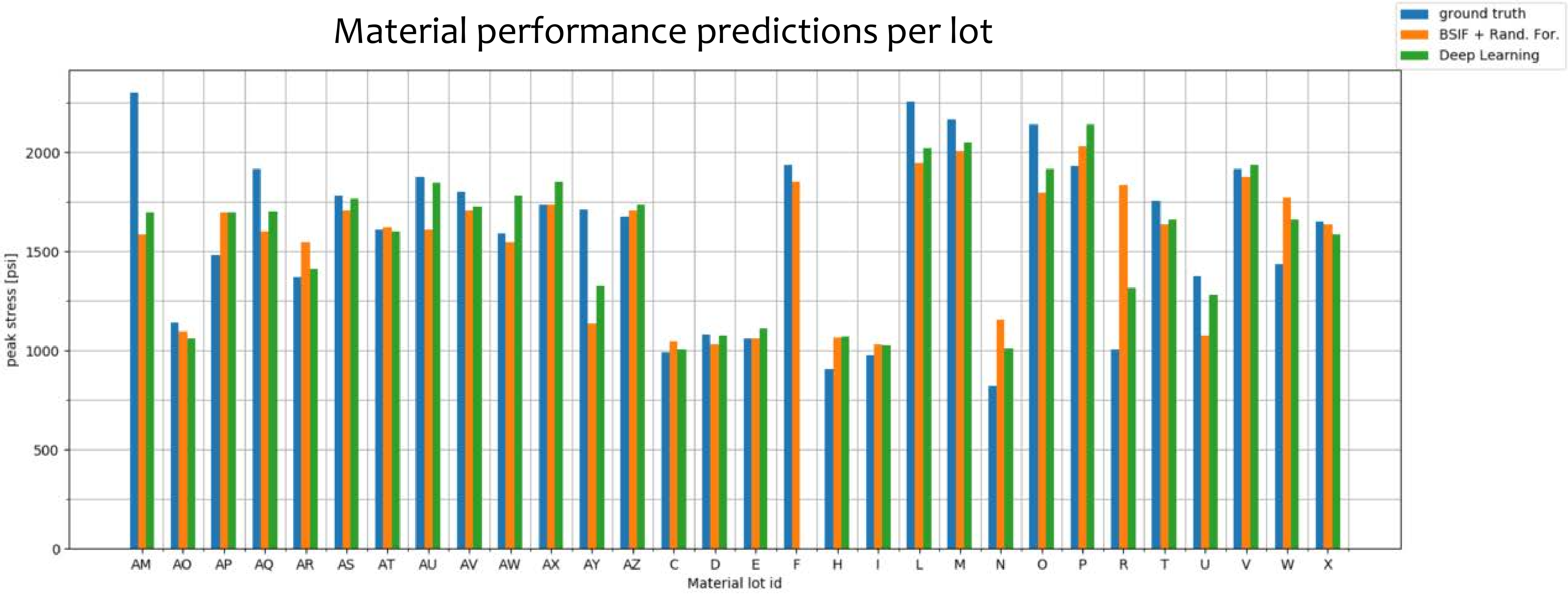
With this model, new lots can be compared to existing or best in class materials prior to extensive testing!

regression

DNN approach performs better than traditional ML

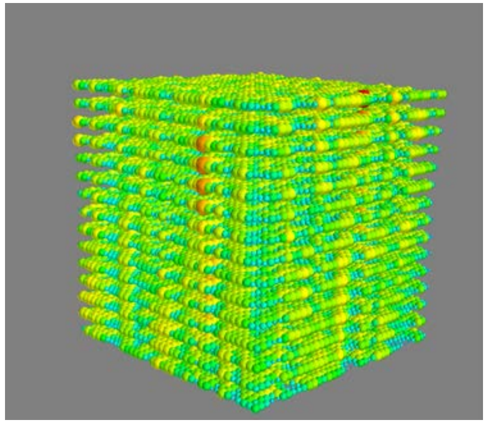
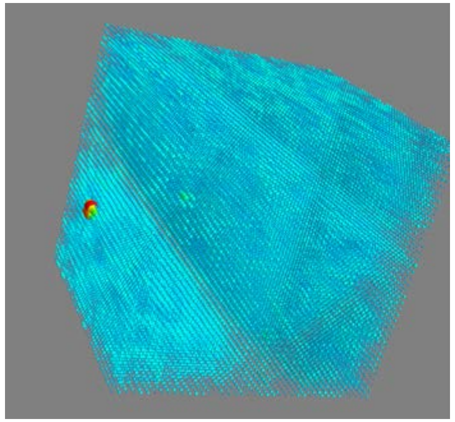
Pros:
DL RMSE: 193 psi
BSIF RMSE: 270 psi

Cons:
Difficult to understand (i.e. how to relate features to physical attributes?)



(All testing performed with leave-one-out cross-validation)

Computed tomography

Sample CT visualizations

- Computed Tomography (CT): 3D reconstruction of material density (in 2D image slices) by way of radiograph projections
- Like SEM, data is relatively inexpensive to acquire

- Pro: CT can reveal information from the 3D structure of the materials
- Pro: Still relatively inexpensive, and multiple lots can be measured at once
- Con: CT data is lower resolution than SEM image data; loses fine detail
- Con: 3D feature extraction is less developed than 2D presently; must find suitable features for classic machine learning; won't have ImageNet equivalent for deep-learning
- Likely, features from CT will augment those from SEM images

Summary and ongoing work

- Machine learning with "classical" computer vision features and regression has been shown to yield promising results for saving time and resources with materials evaluation
- Deep learning currently outperforms the "classical" techniques in terms of prediction accuracy, but may be more difficult to interpret
- We plan to evaluate other key performance metrics in the future and to correlate image/raw-data features with physically measured quantities
- Synthetic data from generative adversarial networks are expected to improve accuracy and help to understand physical attributes from data
- We will use 3D information from computed tomography to augment our predictive capabilities

The end goal is not only produce a predictive performance model, but to enhance our fundamental understanding of the materials so as to produce higher quality feedstock in less time.

Acknowledgments

PI: T. Yong Han

Team members:

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- Shusen Liu
- Nathan Mundhenk
- Emily Robertson

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