Machine learning to analyze deuterium loading patterns during electrochemical experiments

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Abstract

Machine learning is an effective and powerful computational approach that can be successfully applied towards a vast variety of engineering and scientific problems. The key to the approach is to generalize from the observed data to predict the behavior of the system and recognize the correlations and patterns.

We discuss the implementation of machine learning algorithms to analyze experimental electrochemical data obtained in our lab. We use the supervised and unsupervised learning approaches to train the algorithms to recognize patterns in deuterium loading in palladium electrodes. Our analysis reveals important material parameters and experimental conditions that alter loading ratio. Open-source Python-based implementation along with the use of MongoDB relational database makes the data manipulation fast and effective.

More than two decades of collective efforts resulted in significant LENR experimental data pool. Applying learning algorithms for data analysis can provide some important insight to what the nature of the phenomenon is.

Coolescence data

- Research focused on investigating necessary conditions for LENR

  - High deuterium/palladium loading
  - Palladium surface morphology
  - Impurities on palladium surface
  - High deuterium flux in palladium

For details refer to

D. Knies, S.Hamm, O.Dmitriyeva poster presentations

What is Learning?

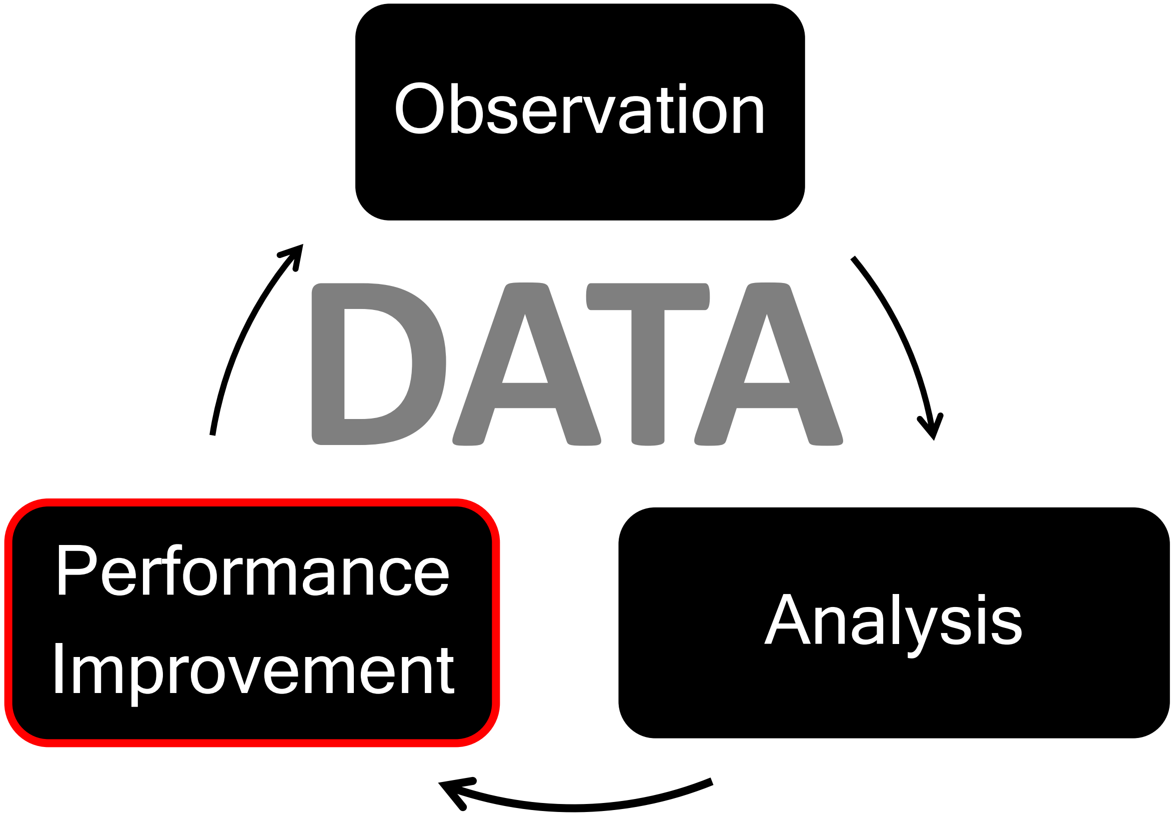
~~Memorization~~

~~Guessing~~

~~Discovery~~

~~Repetition~~

What is Learning?

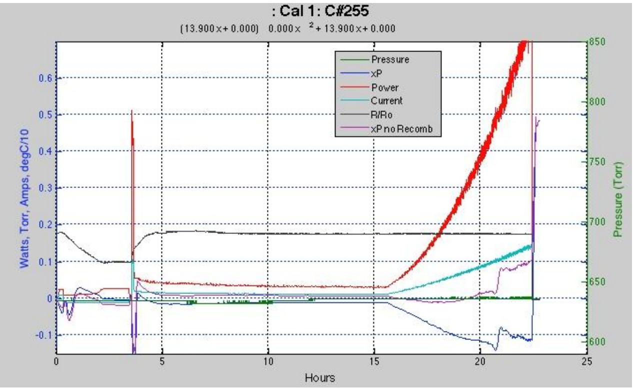


LENR Data

- DATA > 25 years
  - Electrochemistry
  - Plasma discharge
  - Gas-loading
    - Heat generation
    - Chemical elements transmutation
    - Helium production
    - Nuclear particles and gamma-radiation
    - Material properties

Coolescence Data

- Electrochemical experiments 2012-2015:
  - 350 cathodes
  - 35,000 run hours
  - 6,300,000 datapoints including:
    - Temperature
    - Power, Current, Voltage
    - Pressure
    - resistance R/R_0
    - Annealing and etching regimes

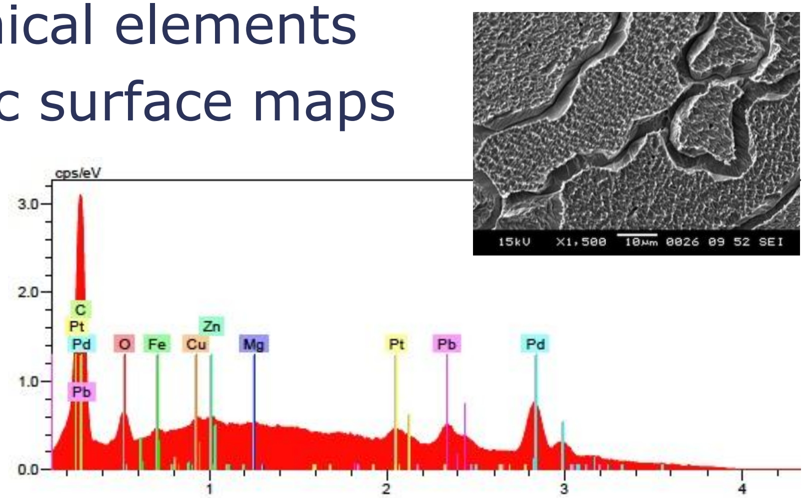


  - Future plans: over 1000 cathodes, 100K run hours

Coolescence Data

More than:

- 2000 SEM images
- 500 EDX spectra on chemical elements
- 600 EBDS crystallographic surface maps
  - boundary grooving
  - grain size
  - crystallographic texture



- Future plans: acquiring ICP-MS for more precise elemental analysis

more DATA is coming!

Machine Learning

- Machine learning is a scientific discipline that explores the construction and study of algorithms that can learn from data to make accurate predictions.

  - Computer vision and object recognition
  - Robot locomotion
  - Bioinformatics
  - Medical diagnosis
  - Natural language processing
  - Computational finance
  - etc…

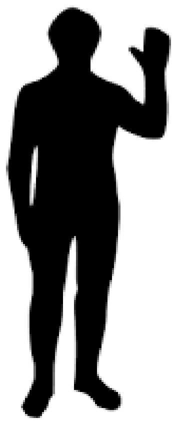
COOLESCENCE

Machine Learning Algorithms

to build predictive models for LENR

Machine Learning to build predictive models

HUMAN



- Provides sets of examples that classifies data
- Asks for predictions

COMPUTER

- Builds model based on given data → hypothesis
- Tests model against unseen data → accuracy
- Makes predictions

Coolescence data analysis

18-Dec	CL#6	5	2.1	2	2				between <100> & <111>			GB, no grooving		
22-Dec	CL#6	6	1.9	1.9	1.96				mid <100> & <111> + <110>			clear GB		
2-Jan	Ingot #3	6	1.82	1.62	1.84									
6-Jan	L149	5	2.05	1.92	1.8	1.93			mostly <100>			no GBG		
6-Jan	IRM 3pass	3	1.9	1.65	1.62									
9-Jan	L148	2	2.03	1.98	1.7				half <100>			no GBG		
9-Jan	L130	4	2	1.7					26% cube			no GBG		

- Features
  - Anneal temperature
  - Grain size
  - EBDS crystallographic orientation
  - EDX chemical elements (surface, bulk)
  - Surface image
  - Source of initial Pd material
  - etc

LABELS
(D_2 loading Yes/No)

FEATURES
(continuous, categorical, binary)

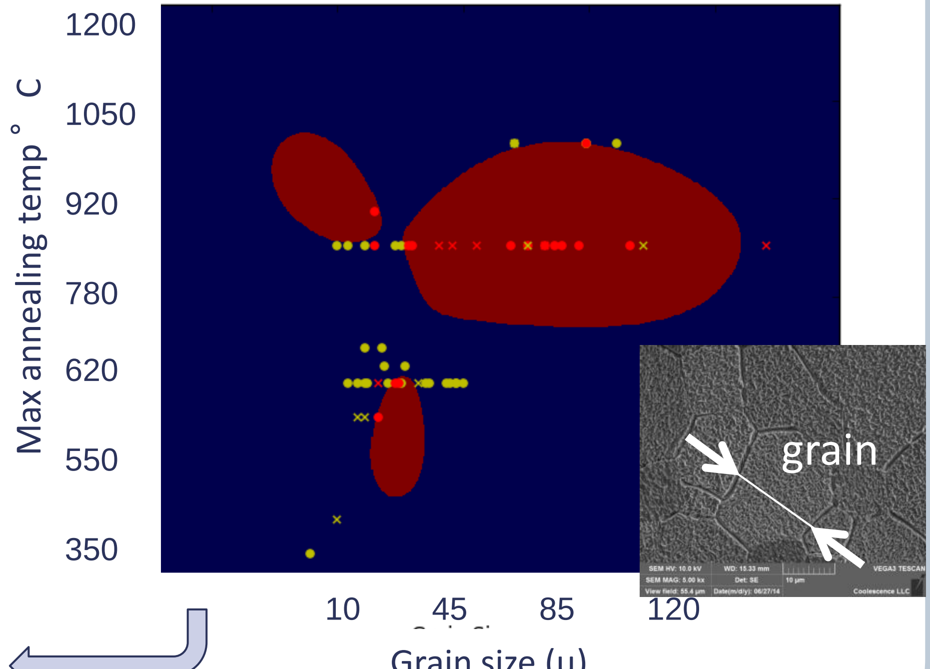
$$\begin{bmatrix} 0 \\ 1 \\ .. \\ .. \\ 0 \end{bmatrix} = f \begin{bmatrix} x_{11}, x_{12} \dots\dots\dots x_{1n} \\ x_{21}, x_{22} \dots\dots\dots x_{2n} \\ \dots \\ \dots \\ x_{350,1}, x_{350,2} \dots x_{350,n} \end{bmatrix}$$

- Labels
  - Loading (1) / Not loading (0)

1. Example: Loading and grain size/annealing temperature

- Does loading depend on grain size and annealing temperature?
- Red - higher loading
- Blue - lower loading

✓59 samples:
24 good loaders D:Pd ≥ 87% , 35 poor loaders < 87%



Predictive model generated by computer using Support Vector Machine algorithm

accuracy of 73%

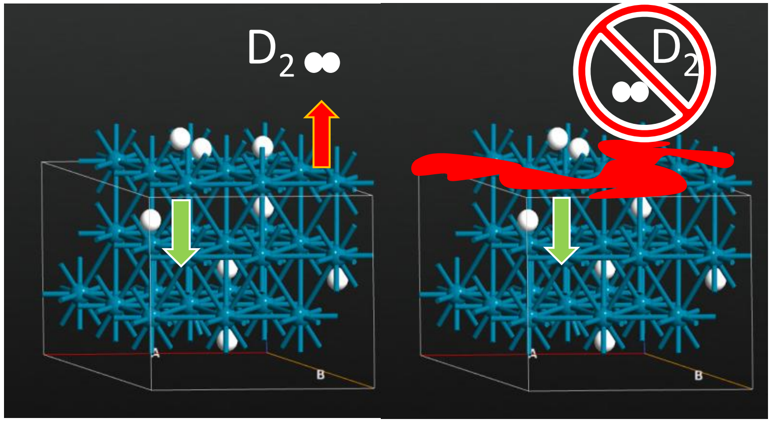
For details on texture processing refer to D. Knies, presentation

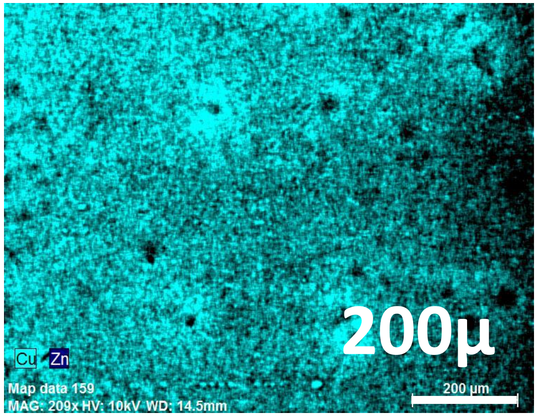
2. Example: loading and effect of surface promoters

Non-uniform coating
of Pd with certain metals:

- Decrease deuterium desorption
- Promotes high levels of bulk loading
- Tested coatings:

  Pb, Cu, Ni, In, Bi, Zn, Fe, Au

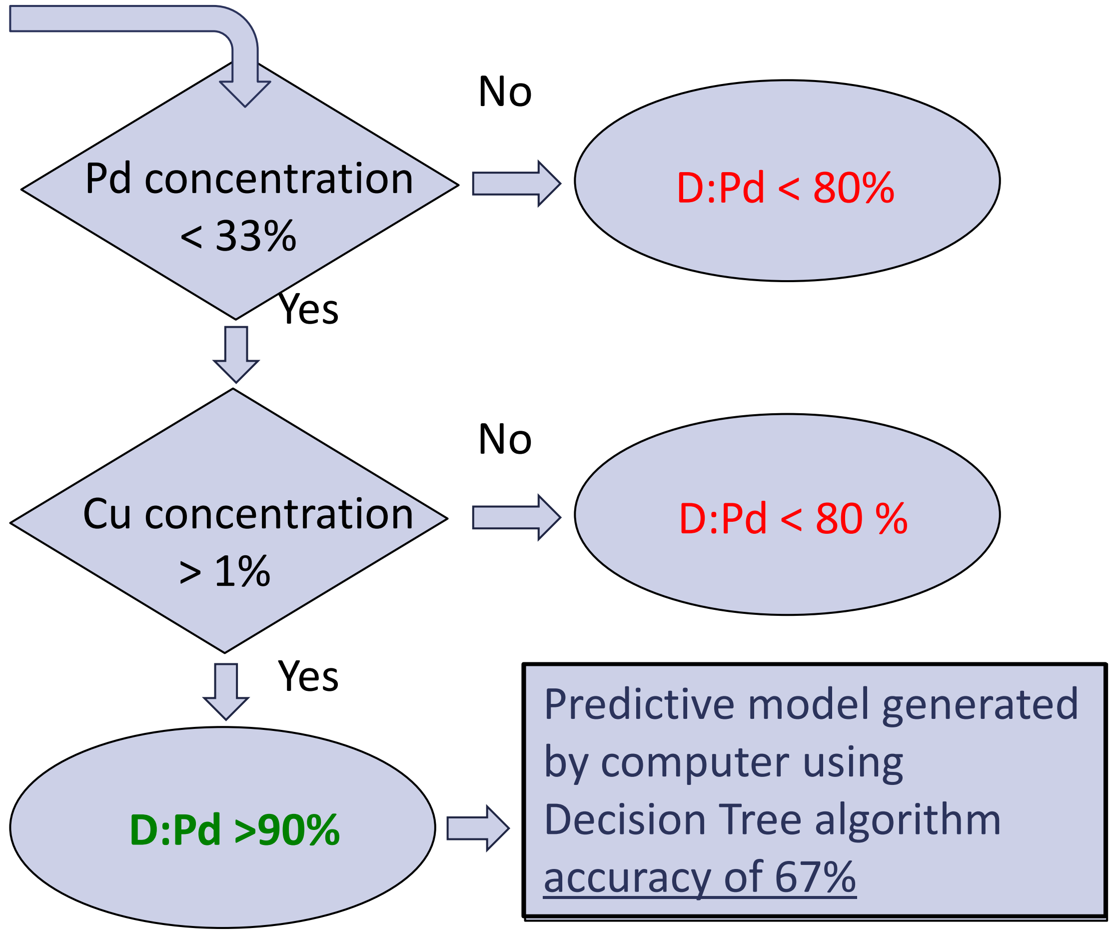




For details on promoting dopants refer to S.Hamm, O.Dmitriyeva poster presentations

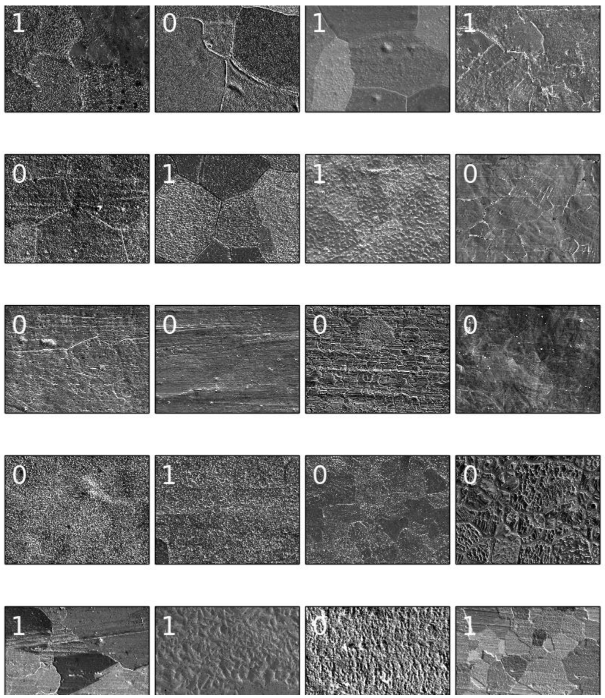
2. Example: Loading and effect of surface promoters

- ✓21 samples
  - 10 good loaders >90%
  - 11 poor loaders < 83%
- ✓EDS 4kV - surface analysis
- ✓17 chemical elements

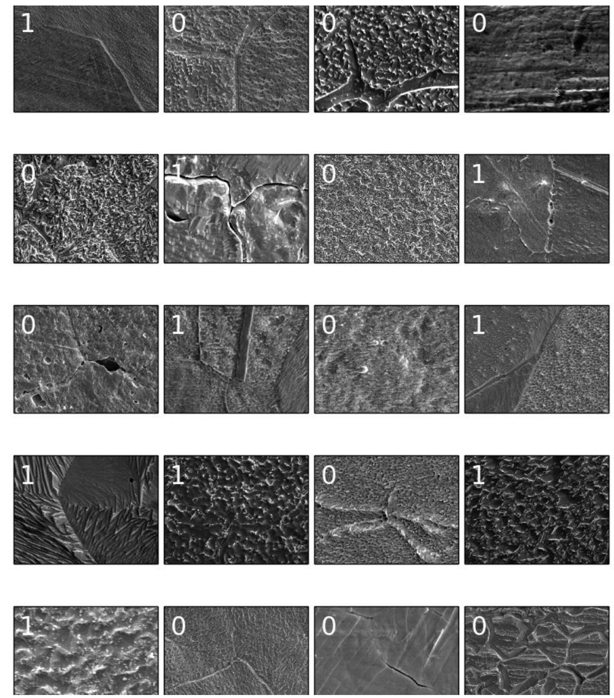


3. Example: loading and surface texture

Magnification 2,000x



Magnification 10,000x

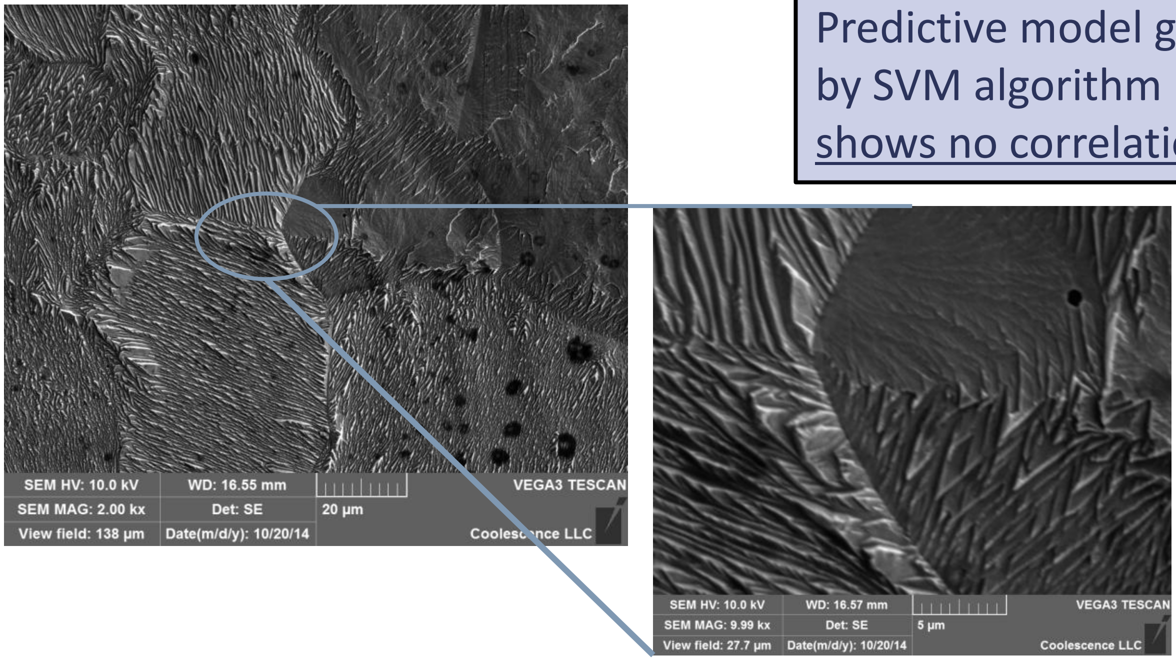


- ✓21 samples (same as for promoting dopants study): good loaders (1) > 90%, poor loaders (0) < 83%
- ✓SEM images are taken at low and high magnification

3. Example: loading and surface texture

Magnification 2,000x
Predictive model generated by SVM algorithm
accuracy 71%

Magnification 10,000x
Predictive model generated by SVM algorithm
shows no correlation



3. Example: loading and surface texture

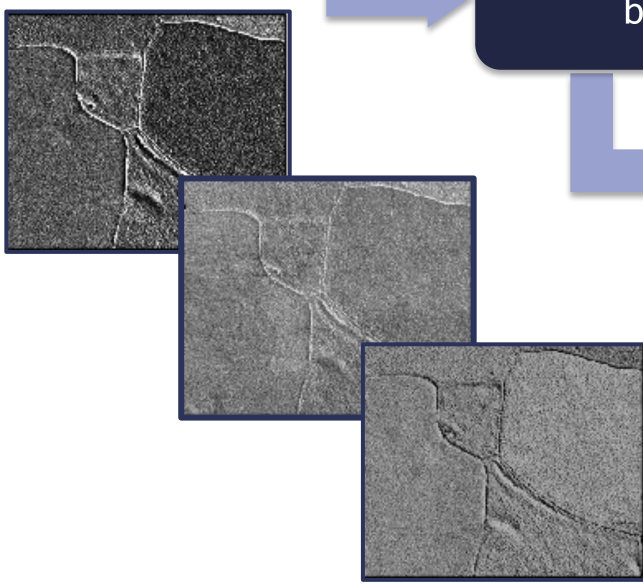
Gray scale 8 bit:
768 x 1024 pixels

Images are normalized in brightness

Independent Component analysis:
786,432 -> 12

21 images:
[21 x 12] matrix

Run time:
under 1 min



Open-Source Machine Learning resources

- scikit - learn* (Python) http://scikit-learn.org/stable/
- R http://www.r-project.org
- Matlab http://www.mathworks.com/machine-learning
- WEKA (Java) http://www.cs.waikato.ac.nz/ml/weka
- ORANGE (Python) http://orange.biolab.si/

....and many more!

* scikit - learn Python library was used for this study.

Conclusions

- Machine Learning is an appropriate technique to analyze assorted experimental data to build predictive models
- ML based analysis of deuterium loading patterns established correlations
  - between grain size boundaries /annealing temperature and loading
  - between impurities on palladium surface and level of loading
- Future work includes cathodes classification based on
  - surface imagery
  - crystallographic orientation (EBDS)
  - electrolyte composition (ICP-MS)