COMPREHENDING NANO-SCALE CORROSION BEHAVIOR USING MULTI- LAYERED PERCEPTRON FOR REGRESSION

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ABSTRACT

- Corrosion impact almost 3.4% of global GDP.
- Complexity and lack of understanding of nucleation process of corrosion.
- Ongoing research suggests crystal features and orientation and electrochemical behavior associated with corrosion.
- Integrated data obtained from scanning electrochemical cell microscopy (SECCM) and electron backscatter diffraction (EBSD) experiment.
- Proposed work exploits multi-layered perceptron (MLP) for regression based deep learning (DL) approach on integrated data to develop a model.
- Developed model can predict corrosion behavior with satisfying accuracy.
- Demonstrate that the behavior are related not only to the grain orientation but also to irregularities of grain surface.

RESEARCH GAP

- Recent research shows a close relationship between crystal orientation and electrochemical properties. [1][3]
- Potential of zero charge (PZC) has been seen to correlate with the local grain crystal orientation. [1]
- Although the relationship was observed, is the orientation information enough to predict the nano-scale electro-chemical behavior?
- Or are there other features that also play role in the corrosion behavior?

CONTRIBUTION

- Image processing-based approach for SECCM and EBSD data integration.
- Development of MLP-Regression model that predicts the corrosion behavior of grains of silver.

HIGHLIGHTS

- **Use of EBSD and SECCM data in the deep learning model.**
- **Corrosion behavior depended not only to grain orientation but also to ups and downs.**
- **Regression model based on deep learning axiom that can predict the electrochemical behavior based on the grain orientation and surface features.**

METHODOLOGY

- Image processing-based matching SECCM datapoints with EBSD orientation and grain information.

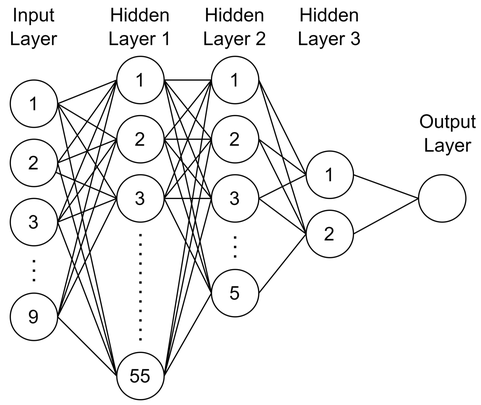


Figure 1 – MLP Structure

MLP Based Regression Model

- Three-layer neural network with limited memory Broyden Fletcher Goldfarb Shanno quasi-Newton algorithm (LBFGS) solver to minimize loss function.
- Developed MLP structure consists of 55, 55, 2 nodes on first, second and third layer, respectively and ReLu function is used as activation function.
- Input features used
  - Position coordinate (XYZ of every datapoint from SECCM experiment)
  - Euler angle (Orientation feature obtained from EBSD)
  - Z gradient with respect to both X and Y
  - Current at pitting condition
- Output response
  - Corresponding voltage at pitting condition

TRAINING SETUP

- Model setup was done in MATLAB environment with Bayseian optimizer for hyperparameter tuning.
- Separate combinations of input features were used for the training to compare the performance.
- Due to the limited availability of the data set three different Current-Voltage pair data obtained from SECCM experiments were used.
- In the preprocessing, outliers present on the data were removed and data was normalized to z-score values.
- From the whole dataset 7 grains obtained from whole experiment were isolated as testing data.
- The remaining dataset was split into 75%-25% training and validation data.
- Finally, to represent the result, predicted vs actual voltage value and IPF are plotted.

RESULTS

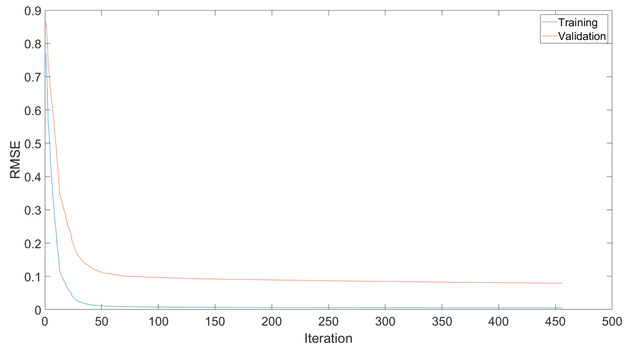


Figure 2 – Training progress using the all-available input features of XYZ, Euler Angle, Gradient of Z with respect to X and Y, and Current value for CV pair

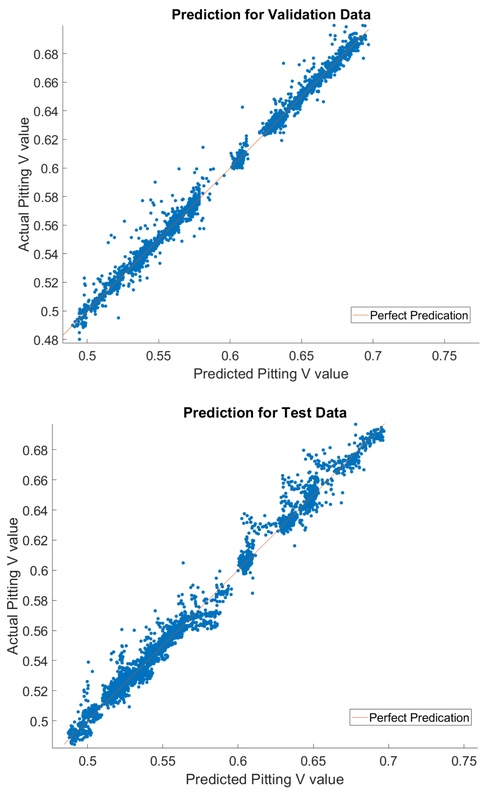
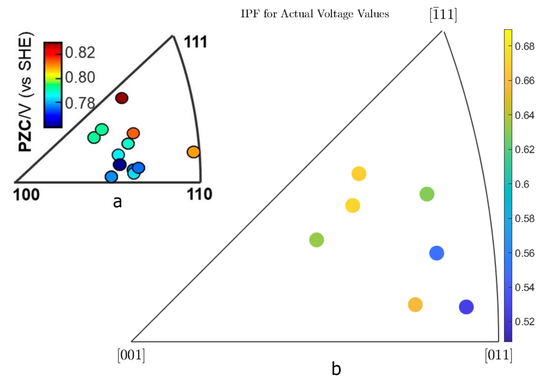


Figure 3 – Actual Pitting Voltage Value vs Predicted Pitting Voltage value for Test (bottom) and Validation data (top)

- Validation and the training RMSE value is decreasing with the number of iteration and showing a proper learning curve of the model.
- Combined use of surface feature and orientation data as input feature showed lower RMSE value and higher prediction accuracy.
- The trained model is able to predict the corresponding value of voltage with **RMSE value** of 0.0794 and **0.1146** for validation and **test** data, respectively.



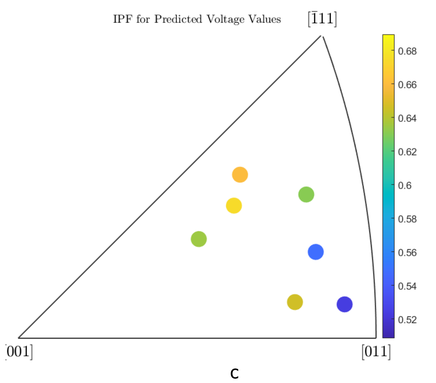


Figure 4 – IPF plot with pitting voltage values represented against the crystal orientation. The color represents the average predicted voltage and position represents the orientation of that grain. (a) Results of PZC/V (Potential of Zero Charge) as a function of orientation. Adapted with permission Ref [1]. Copyright 2020 American Chemical Society. (b) IPF plot with color representing actual voltage value for test data. (c) IPF against predicted test voltage using developed model.

CONCLUSION AND FUTURE WORKS

- Developed MLP model for regression can predict the corrosion behavior with satisfactory accuracy for silver.
- Results indicate behavior are related to grain orientation as well as irregularities in grain surface.
- Can be further expanded to achieve higher accuracy with more data from simulations and experiments.
- Future development towards oracle system that predicts corrosion with full C-V curve for different materials.

REFERENCES

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