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

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INTRODUCTION

Recent research shows a close relationship between crystal orientation and electrocatalytic properties associated with corrosion [1][2]. Specifically, the potential of zero charge (PZC) is seen to correlate with the local grain orientation of a crystal [1]. Although the relationship is observed, a prediction model capable of predicting the nano-scale corrosion behavior is lacking. This work utilizes integrated data obtained from atomic force microscopy (AFM), scanning electrochemical cell microscopy (SECCM), and electron backscatter diffraction (EBSD) experiments for model development.

CONTRIBUTIONS

- Develop a model that can predict voltage during pitting condition by exploiting deep learning (DL) axiom of multi-layered perceptron (MLP) for regression
- Demonstrate that the corrosion behavior is related not only to the grain orientation but also to irregularities of the grain surface.

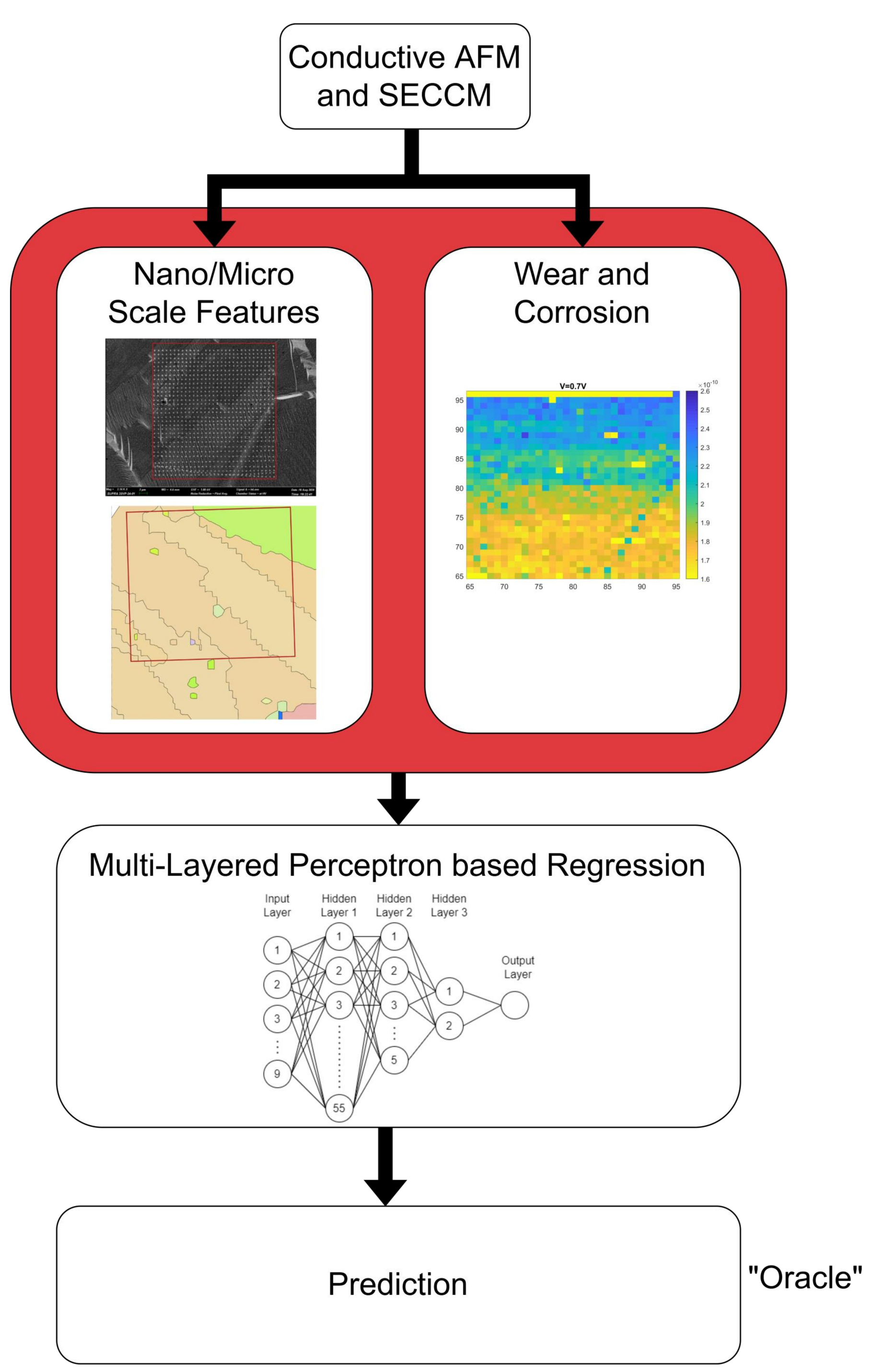

Figure 1 – System diagram

METHODOLOGY

- Image processing-based matching SECCM datapoints with EBSD orientation and grain information.
- SECCM experiment provides the wear and pitting corrosion information seen on the metal surface. And EBSD and SEM data give the nano and microscale features of grains and surface.

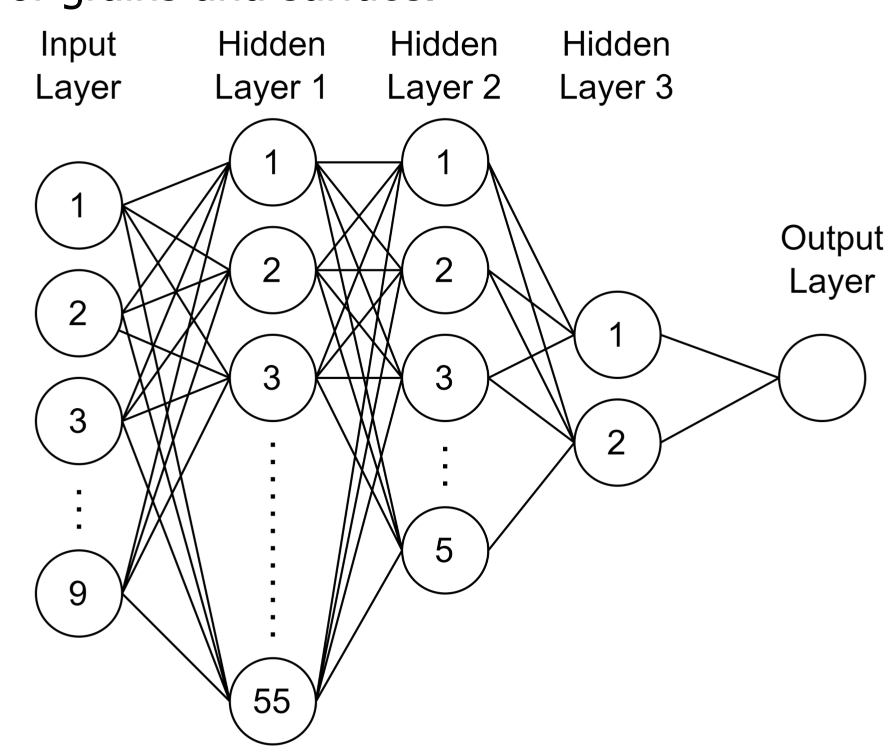

Figure 2 – MLP structure

MLP Based Regression Model

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

TRAINING SETUP

- Model setup is done in MATLAB environment with Bayesian optimizer for hyperparameter tuning.
- Separate combinations of input features are used for the training to compare the performance.
- Three different Current-Voltage (I-V) pairs obtained from SECCM experiments are selected as input data.
- In the preprocessing, outliers present in the data are removed. The data is normalized to the z-score value.
- From the whole dataset, 7 grains are isolated as testing data.
- The remaining dataset is split into 75%-25% training and validation data.
- Finally, to represent the results, the predicted vs actual voltage value is plotted along with Inverse Pole Figure (IPF).

RESULTS

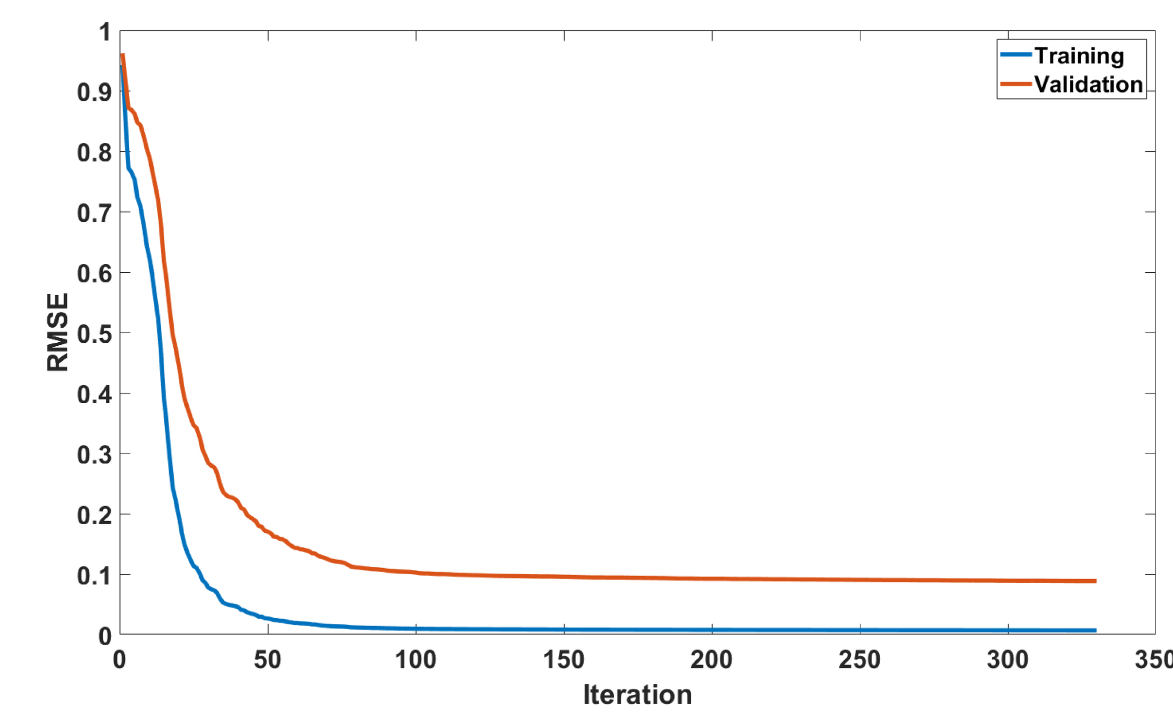

Figure 3 – Training progress using XYZ, Euler Angle, Gradient of Z with respect to X and Y, and Current value from CV pair as input features.

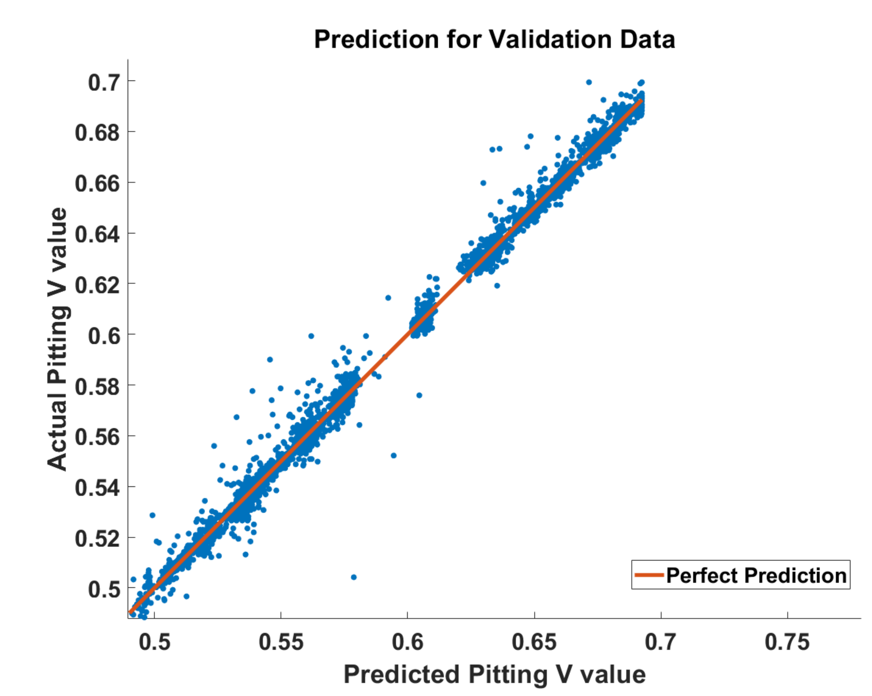

Figure 4 – Actual pitting voltage Value vs predicted pitting voltage value for validation data

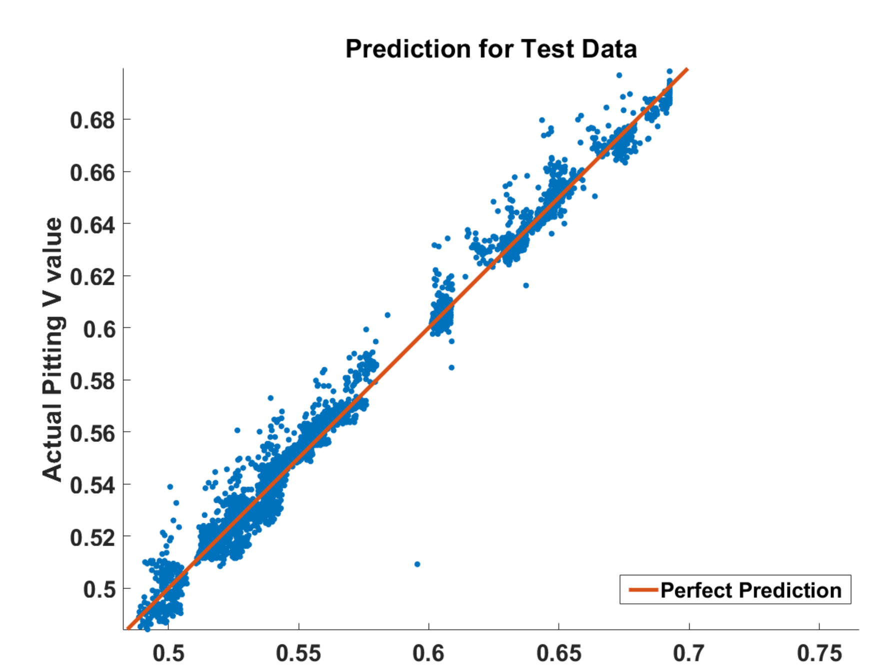

Figure 5 – Actual pitting voltage value vs predicted pitting voltage value for test data

- Validation and the training RMSE value decrease with the number of iterations and shows a proper learning curve of the model.
- Combined use of the surface feature and orientation data as input feature shows lower RMSE value and higher prediction accuracy compared to one or the other.
- The trained model can predict the corresponding voltage value with **an RMSE value** of 0.0886 and **0.1119** for validation and **test** data, respectively.

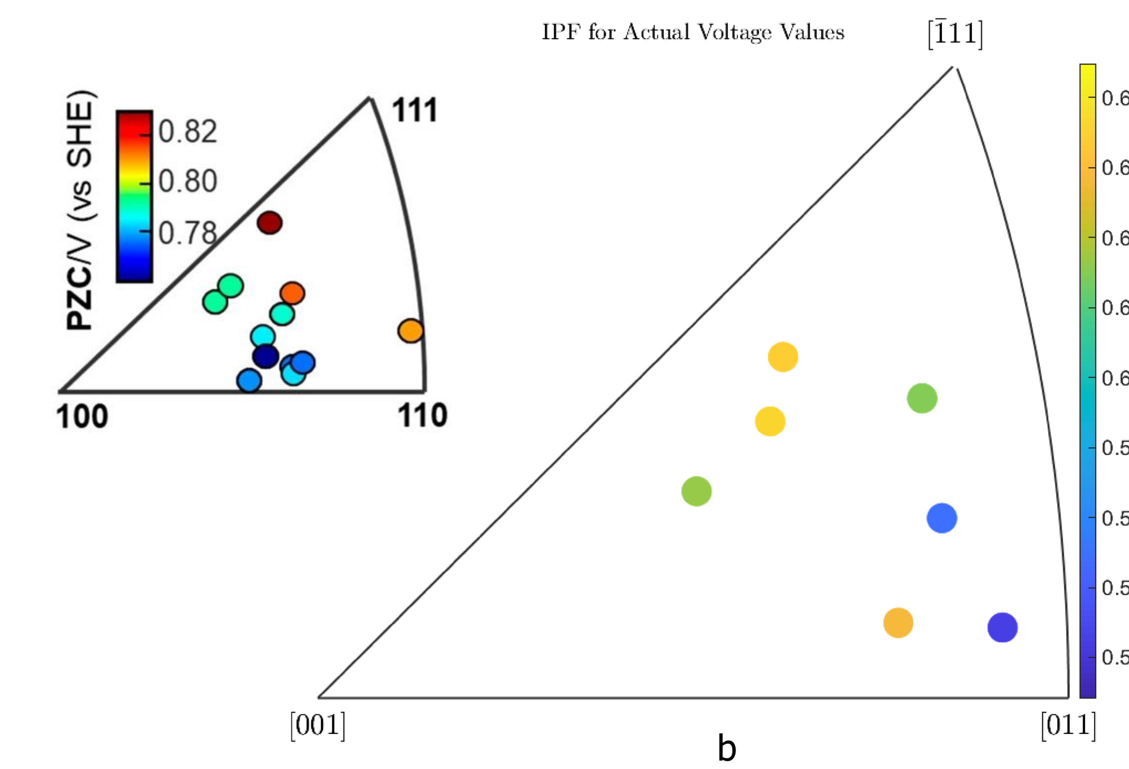

Figure 4 – (a) IPF plot of PZC/V (Potential of Zero Charge) as a function of orientation. Adapted with permission Ref [1]. Copyright 2020 American Chemical Society. (b) IPF plot with color representing actual voltage value at pitting condition for test data.

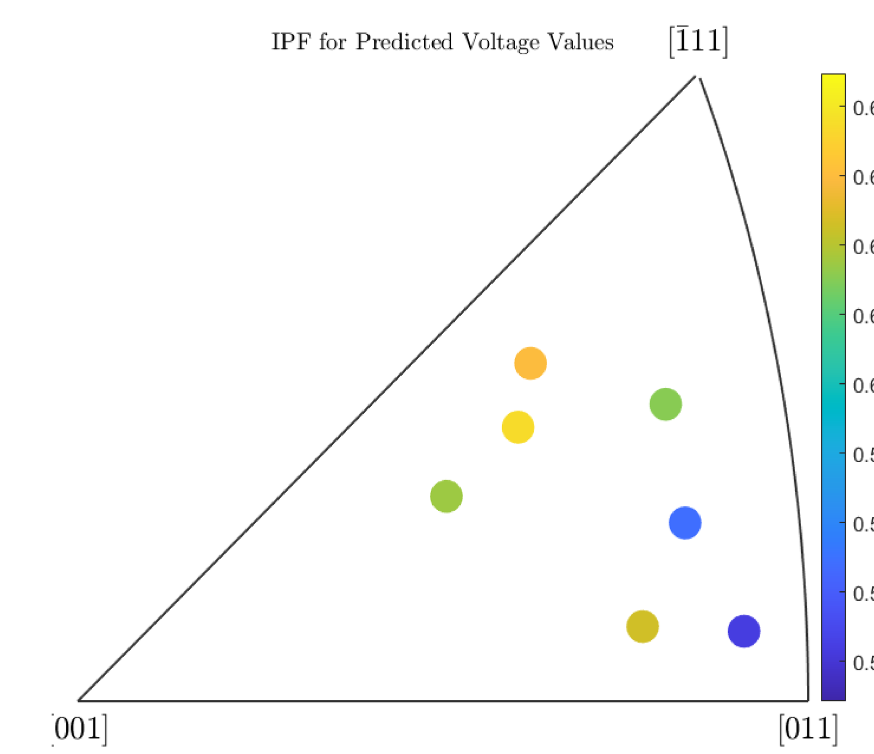

Figure 4 (c) - IPF plot for predicted test voltage using developed model.

CONCLUSION AND FUTURE WORKS

- Developed MLP model for regression has demonstrated that it can predict corrosion behavior with satisfactory accuracy for silver grains.
- Results have indicated the behavior is related to grain orientation as well as irregularities in grain surface.
- Higher accuracy could be achieved with the addition of more data from simulation and experiments.
- An oracle system that predicts corrosion with a complete I-V curve for different materials can be implemented in the future.

REFERENCES

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