# 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][3]. 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 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.

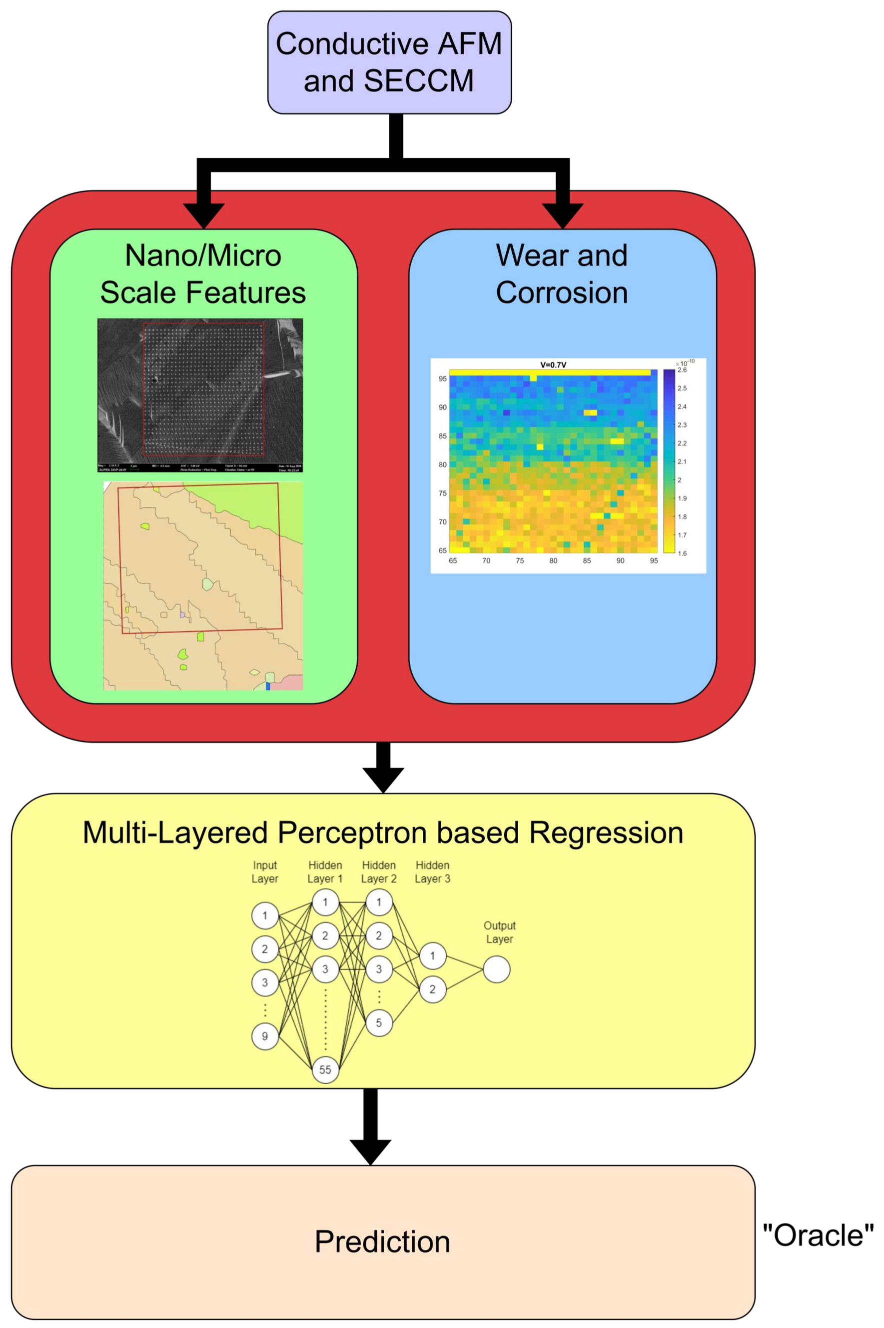


Figure 1 – System diagram

## 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.

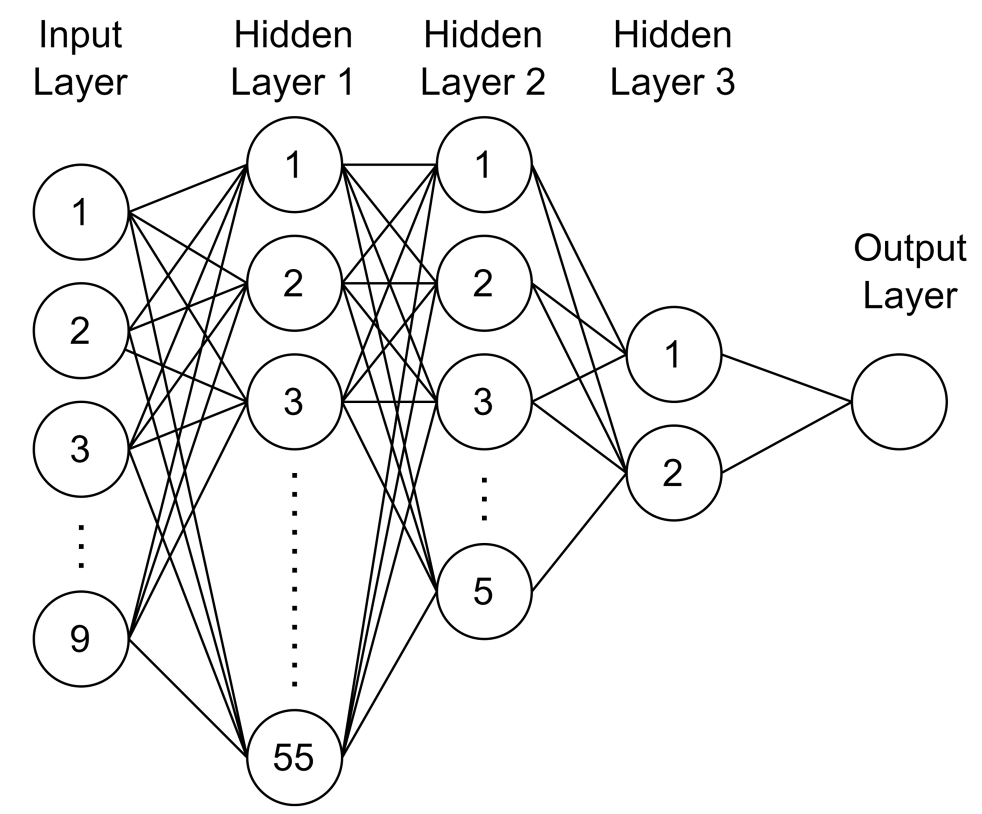


Figure 2 – MLP structure

### 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, 5, 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 environmnt with Bayesian optimizer for hyperparameter tuning.
- Separate combinations of input features are used for the training to compare the performance.
- Three different Current-Voltage 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 IPF.

## RESULTS

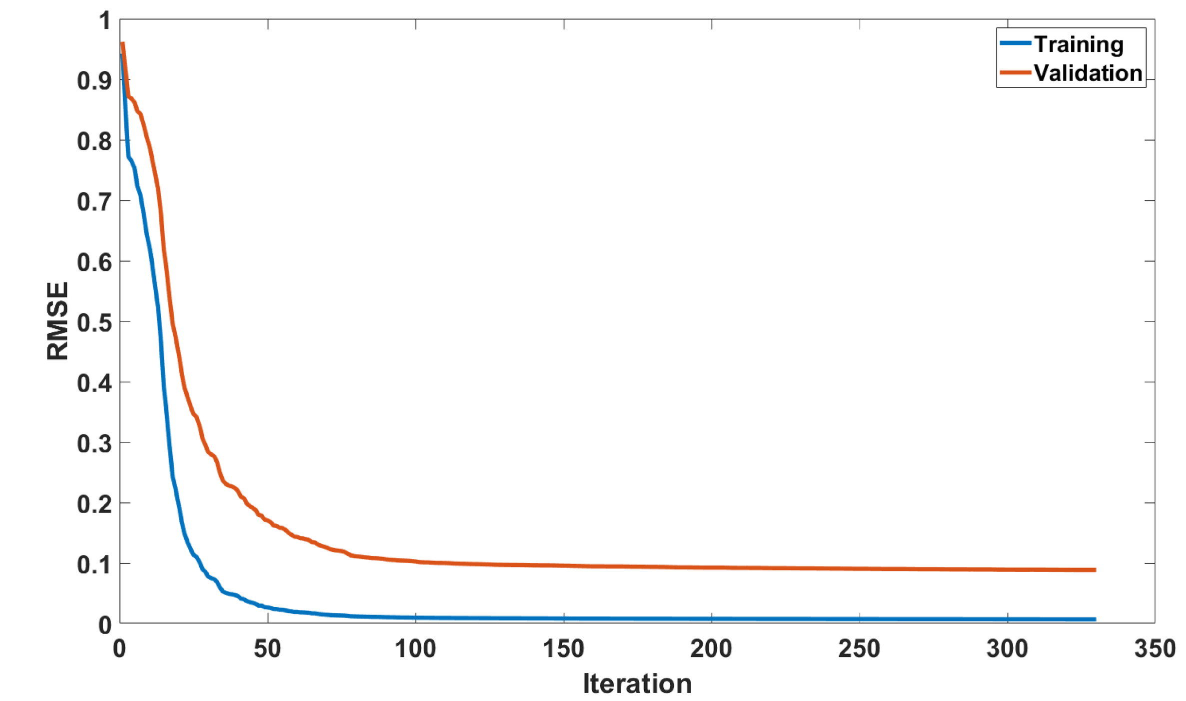


Figure 3 – Training progress using XYZ, Euler Angle, Gradient of Z with respect to X and Y, and Current value from CV pair as input features.

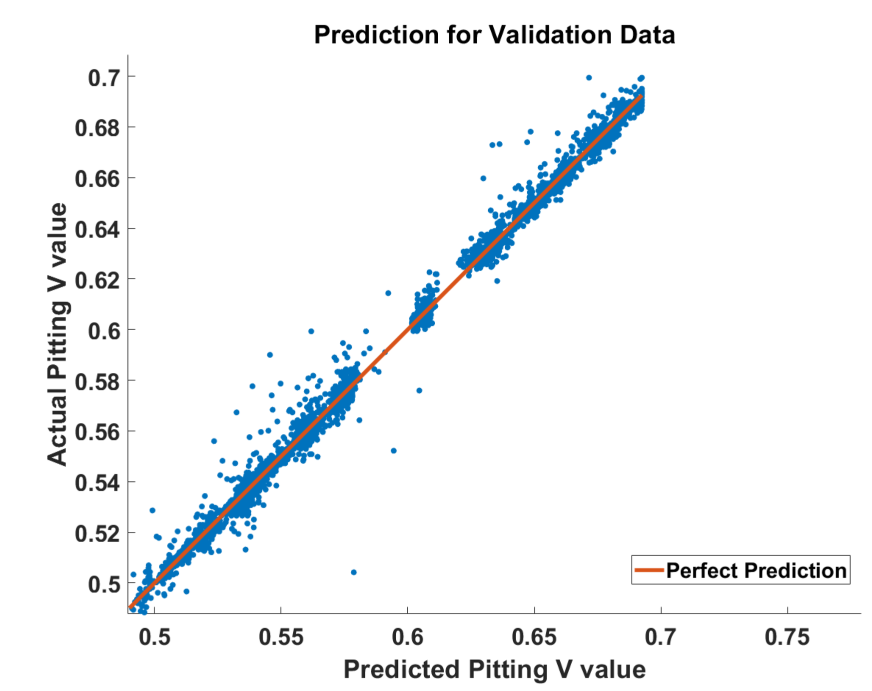


Figure 4 – Actual pitting voltage Value vs predicted pitting voltage value for validation data

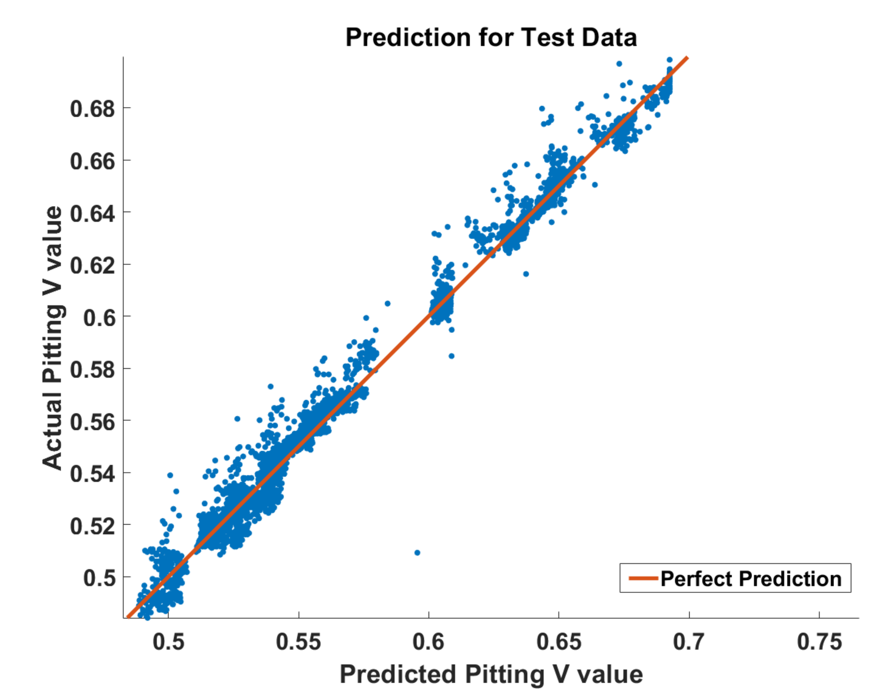


Figure 5 – Actual pitting voltage value vs predicted pitting voltage value for test data

- 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.

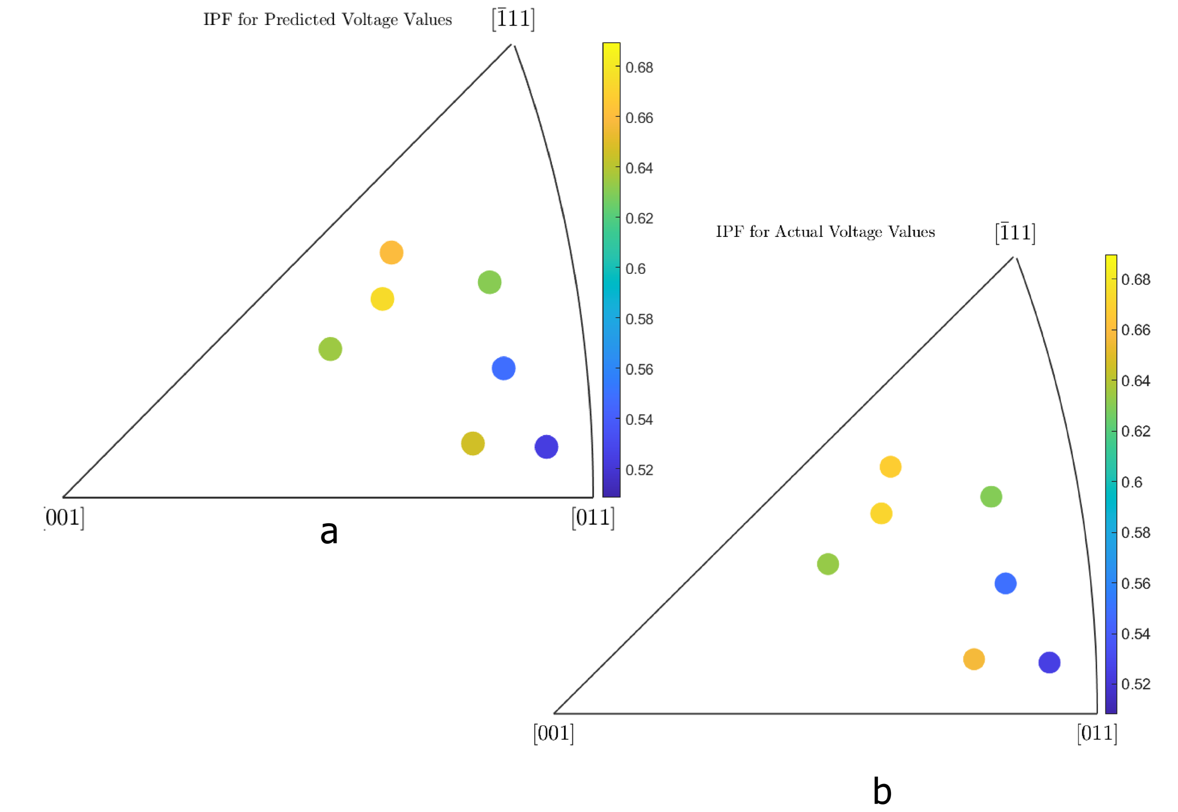


Figure 4 – IPF plot with color representing voltage value at pitting condition for test data (a) predicted voltage value (b) actual voltage value

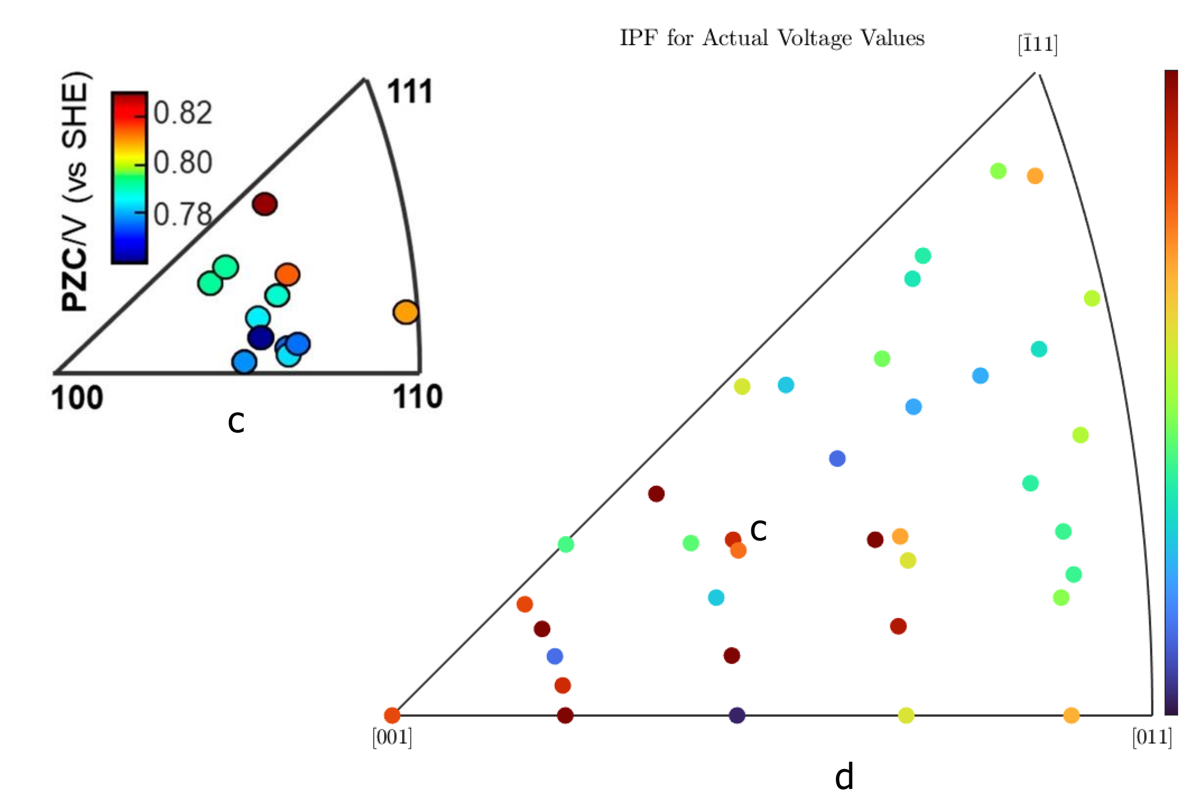


Figure 4 (c) IPF plot of PZC/V (Potential of Zero Charge) as a function of orientation. Adapted with permission Ref [1]. Copyright 2020 American Chemical Society. (d) IPF plot for predicted voltage using developed model for synthetic data.

## CONCLUSION AND FUTURE WORKS

- Developed MLP model for regression has shown 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

[1] Y. Wang, E. Gordon and R. Hang, "Mapping the Potential of Zero Charge and Electrocatalytic Activity of Metal–Electrolyte Interface via a Grain-by-Grain Approach," *Analytical Chemistry,* vol. 92, no. 3, pp. 2859-2865, 2020.

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