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, 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) experiment for model development.

CONTRIBUTIONS

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

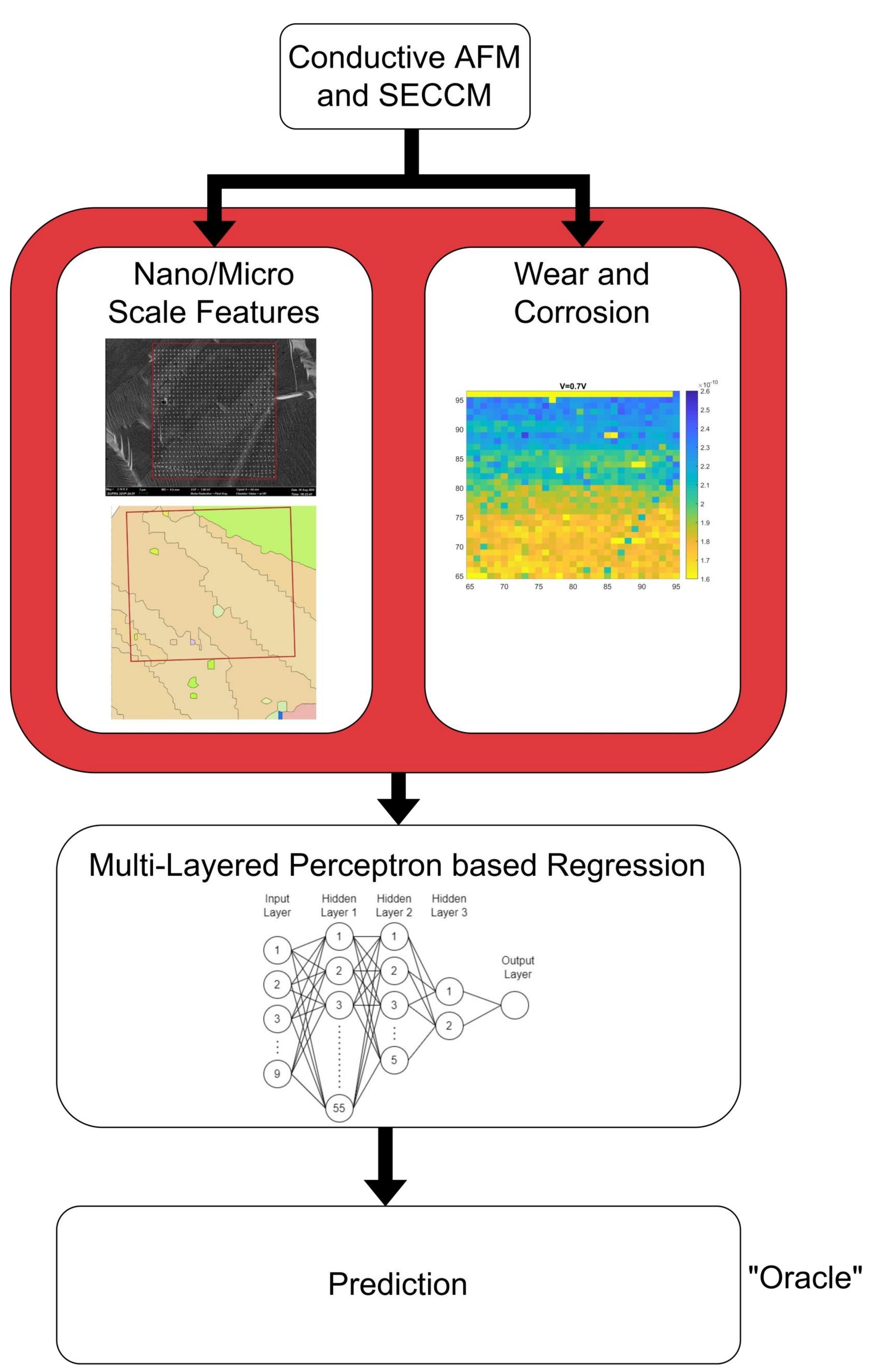

Figure 1 – System diagram

METHODOLOGY

- Image processing-based matching SECCM datapoints with EBSD orientation and grain information.
- SECCM experiment provides the wear and pitting corrosion knowledge of the metal surface and EBSD and SEM data gives the nano and micro scale features of grains and surface.

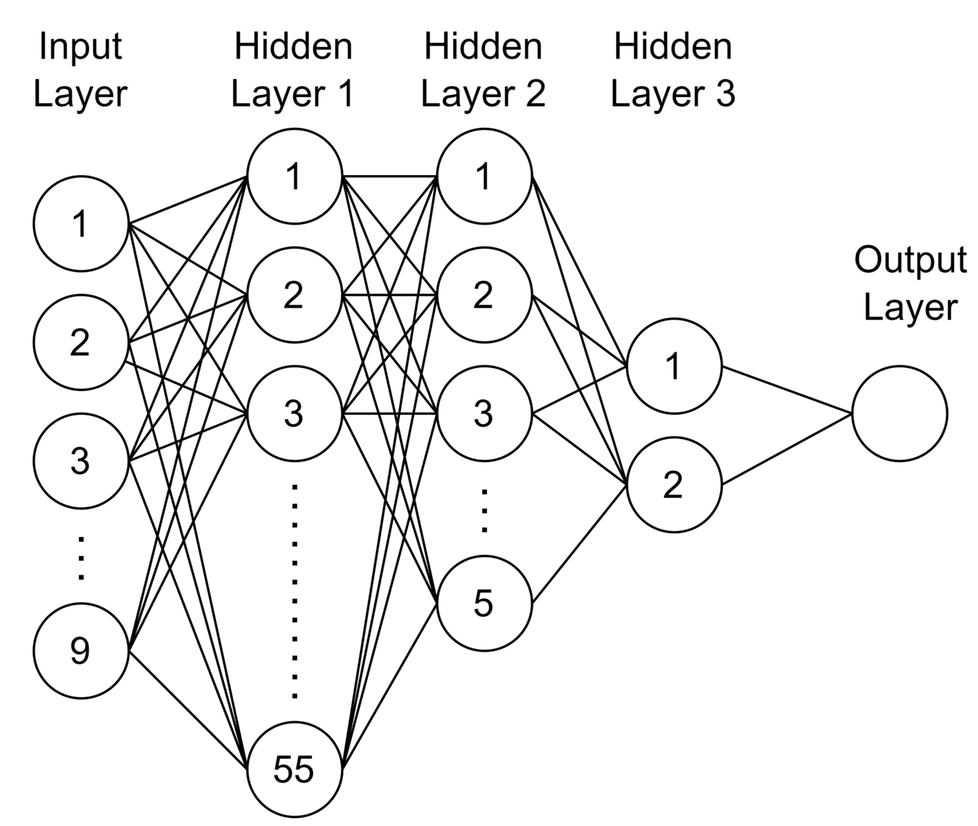

Figure 2 – MLP structure

MLP Based Regression Model

- Three-layer neural network with limited memory Broyden Fletcher Goldfarb Shanno quasi-Newton algorithm (LBFGS) solver to minimize 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)
  - 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 pair obtained from SECCM experiments are selected as input data.
- In the preprocessing, outliers present on the data are removed and data is normalized to z-score values.
- 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 result, predicted vs actual voltage value and IPF are plotted.

RESULTS

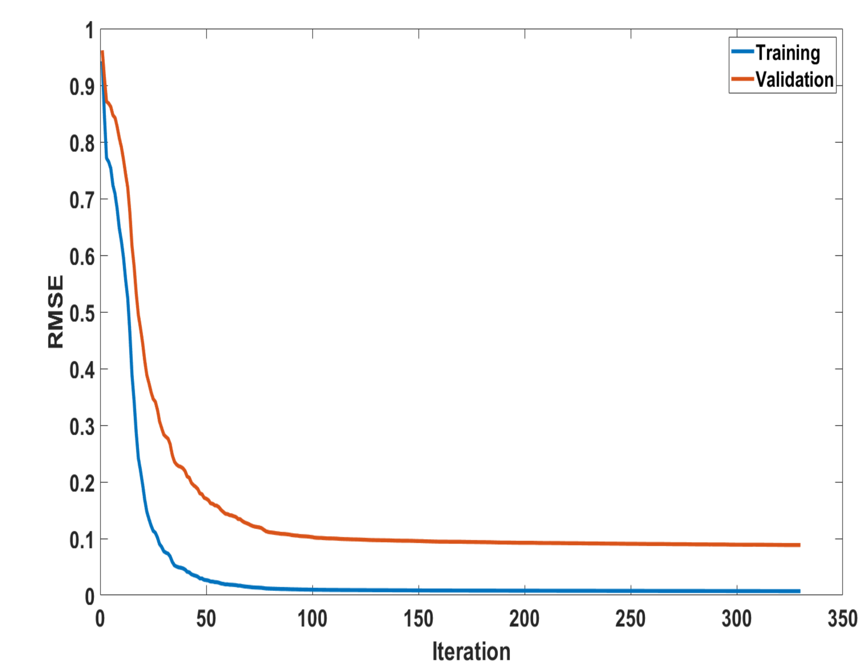

Figure 3 – Training progress using XYZ, Euler Angle, Gradient of Z with respect to X and Y, and Current value from CV pair as input features.

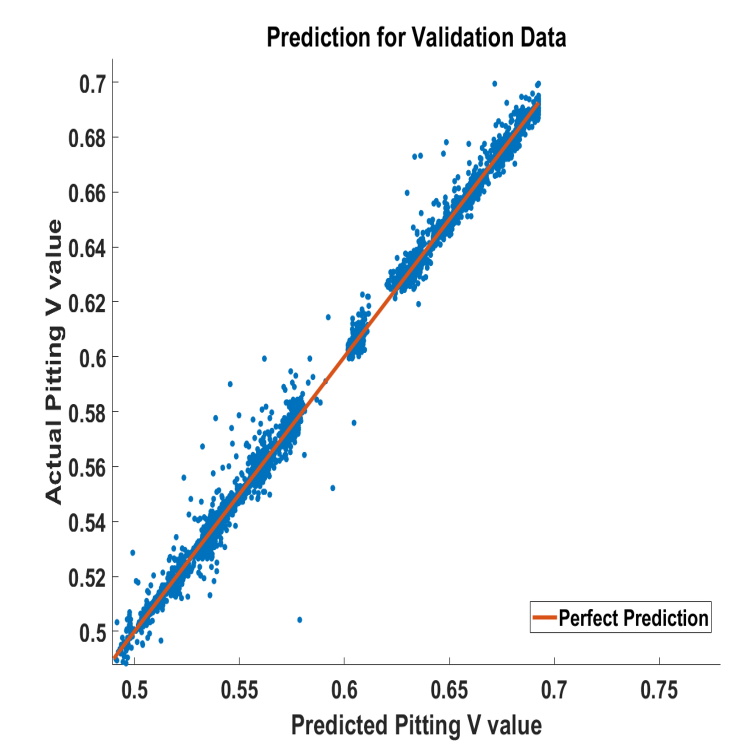

Figure 4 – Actual pitting voltage Value vs predicted pitting voltage value for validation data

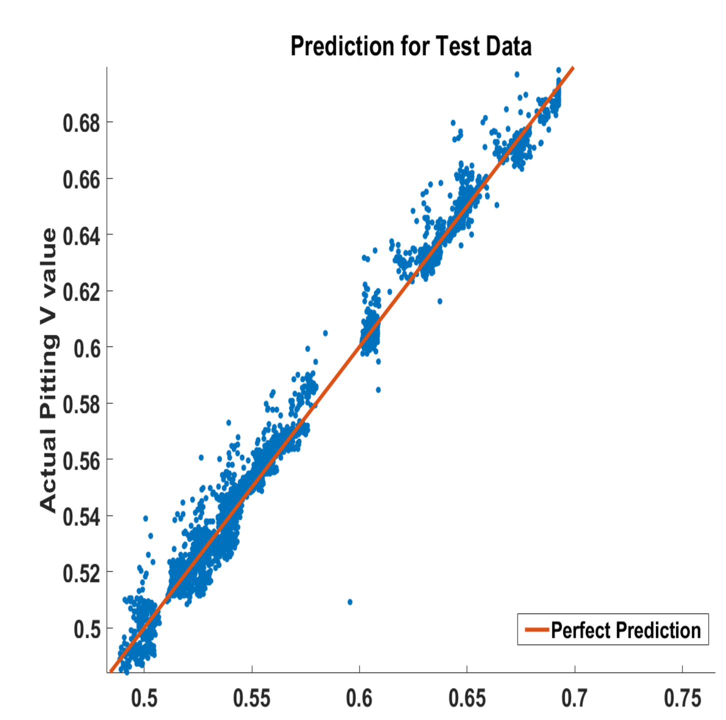

Figure 5 – Actual pitting voltage value vs predicted pitting voltage value for test data

- Validation and the training RMSE value 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 shows lower RMSE value and higher prediction accuracy compared to one or the other.
- The trained model can predict the corresponding value of voltage with **RMSE value** of 0.0886 and **0.1119** for validation and **test** data, respectively.

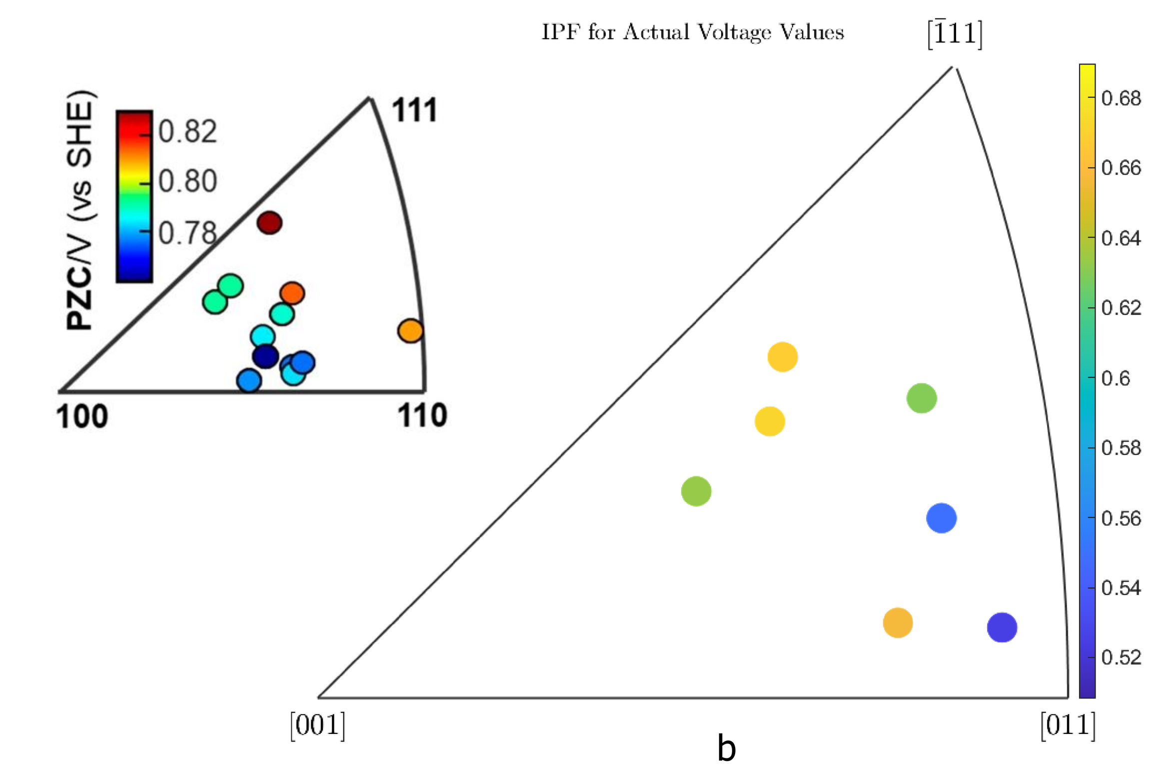

Figure 4 – (a) IPF plot of PZC/V (Potential of Zero Charge) as a function of orientation. Adapted with permission Ref [1]. Copyright 2020 American Chemical Society. (b) IPF plot with color representing actual voltage value at pitting condition for test data.

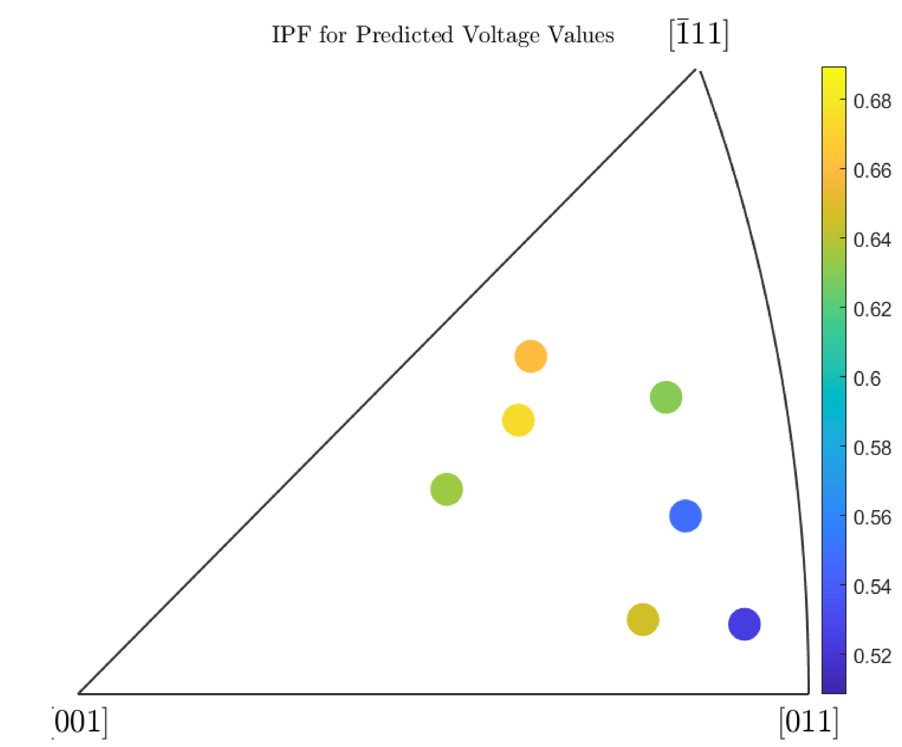

Figure 4 (c) - IPF plot for predicted test voltage using developed model.

CONCLUSION AND FUTURE WORKS

- Developed MLP model for regression can predict the corrosion behavior with satisfactory accuracy for silver grains.
- Results indicate behavior are related to grain orientation as well as irregularities in grain surface.
- Higher accuracy can be achieved with addition of more data from simulations and experiments.
- Future development towards oracle system that predicts corrosion with full I-V curve for different materials.

REFERENCES

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