Real Time Atomic-Scale Mapping of the Relationship between Surface Chemistry and Crystallography to Understand Corrosion

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1. INTRODUCTION

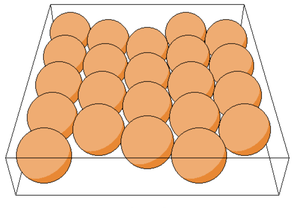
- Catastrophic repercussions of corrosion
  - Accidental injuries and deaths
  - Global economic cost of ~$2.5 trillion
- Increased urgency to develop corrosion-resistant materials and mitigation strategies
  - Ineffective existing corrosion prevention methods
  - Investigation of atomic interactions between metal surfaces and reactive gases remains a challenge
- *Operando* Atom Probe Tomography (OAPT)
  - Real-time nanoscale mapping chemical reactions
  - Display complete crystallographic networks
- Applications of OAPT to understand corrosion
  - Elemental identity of individual atoms on surfaces
  - Dynamic changes between various crystallographic structures
  - New approach to correlate the spatial signal with reaction time
  - Surface reaction kinetics and the crystal structure relationship of material is uniquely revealed
  - Map progression of reactive gas penetration into metal surface forming metal oxide (i.e. corrosion)

2. BACKGROUND

- In this study, we are probing the chemical reaction between Iron metal (Fe(s)) and Oxygen gas (O_2(g))

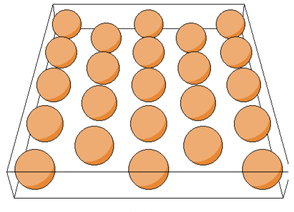
$$XFe(s) + YO_2(g) \rightarrow ZFe_nO_m(s)$$

  - Iron is present in everyday utilities and consumer products in the form of steel
- I hypothesize that rate of oxidation will depend on the arrangement of atoms or crystallographic facets on a surface



(011)

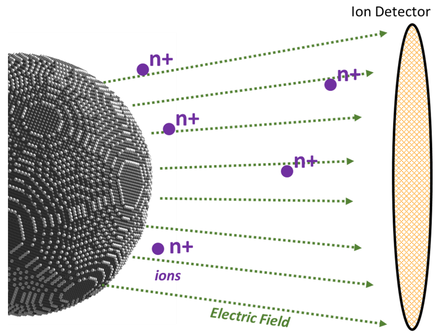
a) Fe {011} facet. The surface is packed with atoms, making this facet resistant to chemical reactions



(222)

b) Fe {222} facet. The atoms are dispersed, making this facet open to oxidation reactions or corrosion

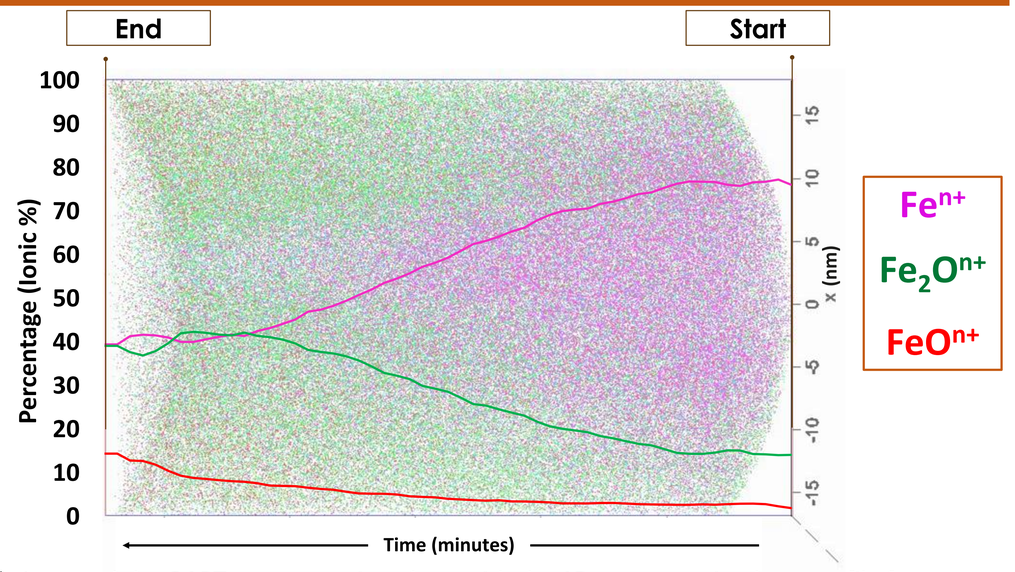
3. OPERANDO ATOM PROBE TOMOGRAPHY (OAPT) PRINCIPLES



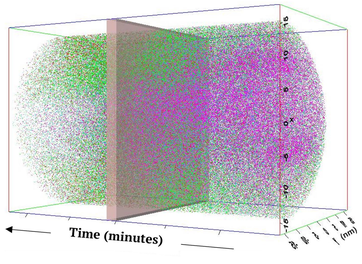
Courtesy to Sten V. Lambeets.

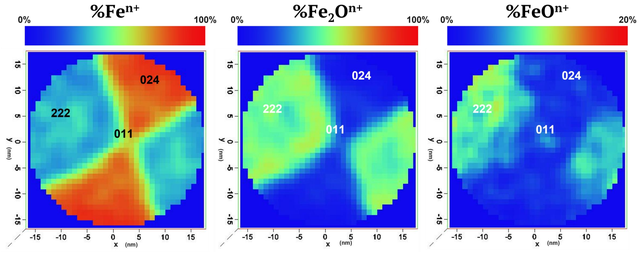
- Field Evaporation
- Time of Flight Mass Spectrometry
- 3D chemical composition and position
  - Reconstruct hemispherical shaped specimen with crystallographic info
- *Operando* mode of analysis
  - Deviates from traditional experiments
    - ✓ Room temperature
    - ✓ Low pressure Oxygen

5. *OPERANDO* RECONSTRUCTION



- I created the OAPT reconstruction along with the 1D concentration heat profile from right to left, showcasing a decrease in Iron and an increase in Iron Oxide concentrations

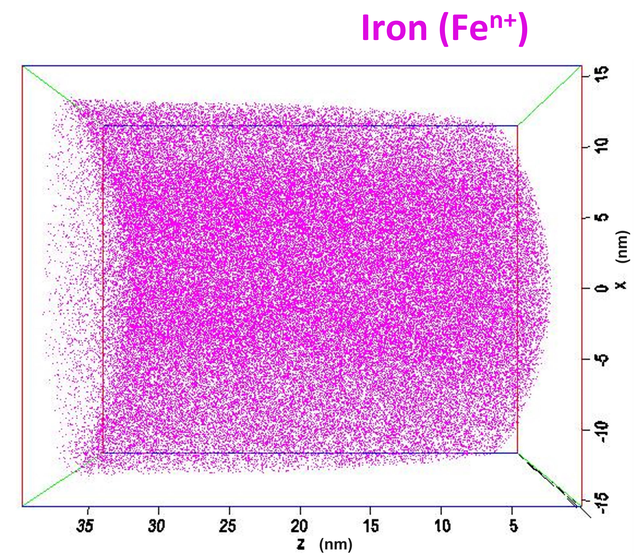




Corrosion Resistant & Susceptible

- I created Regions of Interests (ROI) and associated 2D concentration heat maps for Iron and Iron Oxides, labeled with the major surface facets, along the time axis
  - I created a Python script connecting the concentration heat maps from beginning to end of the experiment or along the time axis
  - Results support the hypothesis that different surface facets on materials will result in different rates of oxidation as shown by the inhomogeneous distributions

4. 3D DATA RECONSTRUCTION



- Integrated Visualization and Analysis Software (IVAS)
  - 3D point could map with chemical identity
- Challenge to correlate the z-axis to a function of time for *Operando* Atom Probe Tomography

6. CONCLUSION

- Metal oxidation reaction rates are dependent on the crystallographic structures on a surface as demonstrated by the experimental results
- The novel OAPT technique can be used to understand the chemical and physical properties of a material
- Efforts to investigate surface gas reaction at the atomic scale will allow for the development of better corrosion mitigation methods

ACKNOWLEDGEMENTS

The work presented here was supported by the LDRD program at the Pacific Northwest National Laboratory (PNNL), which is operated for the U.S. DOE by Battelle Memorial Institute. A portion of this research was performed using facilities at the Environmental Molecular Sciences Laboratory, a national scientific user facility sponsored by the DOE Office of Biological and Environmental Research and located at PNNL.

Thank you to Daniel E. Perea, Sten V. Lambeets, and Mark G. Wirth for their guidance and support. Thank you to Diane L. Showers, Scott Lea, and the Office of STEM Education Staff, Nancy Roe, Juan Lopez, and Nicole Castilleja-Bentley for their support and encouragement throughout the research project.

This work was supported in part by the U.S. Department of Energy, Office of Science, Office of Workforce Development for Teachers and Scientists (WDTS) under the Community College Internship (CCI) program.