Understanding Corrosion in 4D

A Multidisciplinary University Research Initiative

Executive Summary

The critical importance of corrosion has been known for centuries as have ways to try and reduce it. However, much of our current knowledge is the phenomena from the mesoscale down to several nanometers. In other areas there has been an explosion of tools to image materials at the atomic scale, as well as accurately calculate their behavior. For instance, not only can single atoms be imaged, their chemical state can be measured. Modern ab-initio methods such as density functional theory are now starting to be able to handle materials such as transition metal oxides, where older functionals can go catastrophically wrong.

The intent of this five year project funded by the Office of Naval Research is to bring the full power of these new tools to bear on corrosion at the atomic scale to unravel how the nanoscale structure influences the properties in 4D. We hypothesize that the near-surface selvedge region microstructure at the nano to mesoscale plays a critical role. We know that the selvedge region, that is the area near the surface where properties are significantly different from the bulk material matters, but we do not understand the details. What transient and perhaps metastable oxides form on NiAlCr alloys? Are they the same in the different phases and how do we understand and accurately model this? Does the temperature dependence of oxygen diffusion lead to MoO_x oxides in the bulk material and phase boundaries in the selvedge region, and what are the kinetics? What is it about dopants in alloys changing aqueous corrosion, is it changes in the Fermi energy of the oxide or do segregation and diffusion also matter?

Our specific target is to understand in detail the early-stage oxidation and aqueous corrosion in three selected model systems. We believe that a comprehensive experimental and theoretical attack on the details will enable us to understand what matters, what does not, and lay the basis for a paradigm shift in improvements of corrosion-resistant materials. Our specific targets are:

- NiCrAl alloys, a classic two-phase high-temperature alloy with alumina or chromia protection.
- MoSiB alloys, a new class of alloys for higher-temperature applications with a self-forming glass protective coating.
- Aqueous corrosion resistant materials with dopants effecting oxide growth that are used for many current marine applications.

The problem requires a broad attack exploiting unique methods and instrumentation. For this purpose we have assembled a multidisciplinary team involving faculty from Northwestern University, the University of Akron, the University of California at Los Angeles, the University of Virginia and the University of Wisconsin-Madison.

We believe the same methods can be applied to a wide range of other corrosion related problems.

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