Understanding the role of Chloride in Corrosion: DFT, TEM and Morphological Instabilities

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Abstract

It has been known for at least a century that chloride has a major effect on corrosion, often increasing the rate of attack by an order of magnitude or more. This has serious consequences, not just for corrosion in sea water but also within humans; they have similar chloride ion levels. The literature is full of conflicting models each developed with particular approaches focusing on one aspect of the problem, rarely looking at the larger picture.

The focus of this talk will be to show that the different conflicting models are not in fact conflicting. Density functional theory calculations show that chloride plays a critical role in disrupting the hydrogen bonding networks at oxide surfaces by replacing chemisorbed hydroxide. This leads to a reduction in the surface free energy which promotes morphological instabilities, these later conclusions being supported by transmission electron microscopy and atom probe tomography results.

Biography

Laurence Marks is a Professor in the Department of Materials Science and Engineering at Northwestern University. While over the years he has published extensively in electron microscopy, he has also worked in many other areas including nanoparticles, oxide surface science, heterogeneous catalysis, nanotribology, density functional theory algorithms and more recently flexoelectric phenomena and corrosion/oxidation. He has supervised 49 PhD students and 26 postdoctoral students, with more than 380 published refereed papers. He was the recipient of the Burton Medal of the Electron Microscopy Society of America in 1989, the 2015 Warren Award of the American Crystallographic Association and the 2017 International Surface Structure Prize. He always tells his students to follow the science, not the electron.