

The core of corrosion

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Typically, the process of corrosion has been studied from the metal side of the equation.

(Phys.org) —Anyone who has ever owned a car in a snowy town – or a boat in a salty sea – can tell you just how expensive corrosion can be.

One of the world's most common and costly [chemical reactions](#), [corrosion](#) happens frequently at the boundaries between water and [metal surfaces](#). In the past, the process of corrosion has mostly been studied from the metal side of the equation.

However, in a new study, scientists at the Center for Nanoscale Materials at the U.S. Department of Energy's Argonne National Laboratory investigated the problem from the other side, looking at the dynamics of water containing dissolved ions located in the regions near a metal surface.

A team of researchers led by Argonne materials scientist Subramanian Sankaranarayanan simulated the physical and chemical dynamics of dissolved ions in water at the atomic level as it corrodes [metal oxide](#) surfaces. "Water-based solutions behave quite differently near a metal or oxide surface than they do by themselves," Sankaranarayanan said. "But just how the chemical ions in the water interact with a surface has been an area of intense debate."

Under low-chlorine conditions, water tends to form two-dimensional ordered layers near solid interfaces because of the influence of its strong hydrogen bonds. However, the researchers found that increasing the proportion of [chlorine ions](#) above a certain threshold causes a change in which the solution loses its ordered nature near the surface and begins to act similar to [water](#) away from the surface. This transition, in turn, can increase the rate at which materials corrode as well as the freezing temperature of the solution.

This switch between an ordered and a disordered structure near the [metal](#) surface happens incredibly quickly, in just fractions of a nanosecond. The speed of the chemical reaction necessitates the use of high-performance computers like Argonne's Blue/Gene Q supercomputer, Mira.

To further explore these electrochemical oxide interfaces with high-performance computers, Sankaranarayanan and his colleagues from Argonne, Harvard University and the University of Missouri have also been awarded 40 million processor-hours of time on Mira.

"Having the ability to look at these reactions in a more powerful simulation will give us the opportunity to make a more educated guess of the rates of corrosion for different scenarios," Sankaranarayanan said. Such studies will open up for the first time fundamental studies of corrosion behavior and will allow scientists to tailor materials surfaces to improve the stability and lifetime of materials.

More information: Sanket Deshmukh, Ganesh Kamath, Shriram Ramanathan, and Subramanian K. R. S. Sankaranarayanan, "Chloride ions induce order-disorder transition at water-oxide interfaces" *Phys. Rev. E* 88, 062119 (2013) [5 pages] [DOI: 10.1103/PhysRevE.88.062119](https://doi.org/10.1103/PhysRevE.88.062119)

Provided by Argonne National Laboratory

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