# SIMULATION-LED STRATEGY FOR CORROSION PREVENTION

Costing billions of dollars annually, corrosion is everyone's problem. Fundamental research in corrosion science at the Naval Research Laboratory will enable scientists to design materials that inherently prevent corrosion.

BY JENNIFER A. SEGUI

Corrosion is a complex multiphysics problem that is currently under investigation by Siddiq Qidwai, a mechanical engineer, and his colleagues at the Naval Research Laboratory (NRL) in Washington, D.C. "In the long run, the success of our research will result in microstructure-corrosion correlations that will enable material designers to include or preclude certain features in the development of new corrosion-resistant materials," explains Qidwai.

A 2011 National Academy of Sciences report from the National Research Council in the U.S. states that a "lack of fundamental knowledge about corrosion and its application to practice is directly reflected in the high societal cost of corrosion." Based on figures reported in December 2010, as much as 600 billion dollars, that is 2 to 4 percent of the U.S. gross national product, were spent to repair or prevent corrosion damage.

The transportation industry including sea, air, and ground transport is particularly affected by corrosion where maintenance costs to preserve passenger safety and vehicle longevity are extremely high. "For the Navy specifically, corrosion is the number one maintenance problem," says Qidwai.

## SMALL GRAINS WITH BIG IMPACT

Pitting corrosion occurs in a metal when electrochemical reactions and mass transport in an adjacent electrolyte solution result in localized loss of material, as shown in Figure 1. "The pit keeps growing and eventually the material or component will fail under load," says Qidwai, emphasizing the effect that corrosion can have on the strength or integrity of a material.

Qidwai and his colleagues have come up with an innovative and comprehensive approach to better understand pitting corrosion. "We are modeling the growth of corrosion pits in metals in a seawater environment," he explains. "The microstructure of the metal has not been the focus of attention in previous work and consequently the challenges associated with irregular growth

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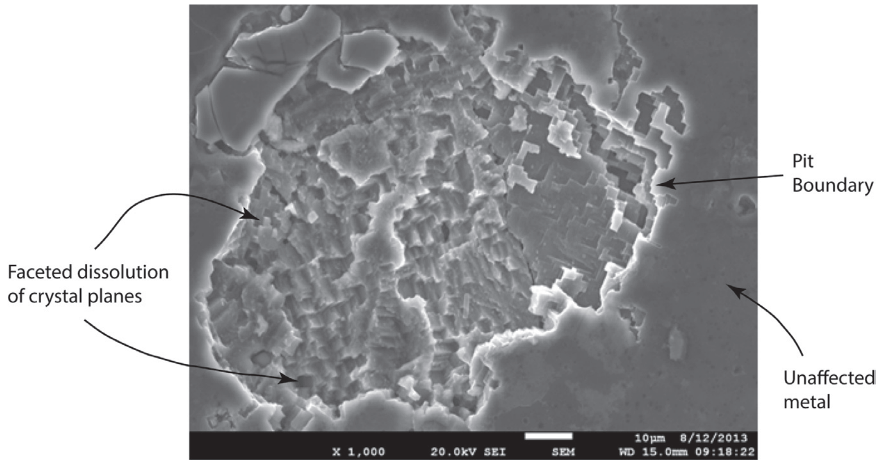


FIGURE 1. Example of pitting corrosion (top-down view) in an aluminum alloy clearly demonstrates the characteristic localized loss of material. The formation of pits can reduce the strength of a material. *Image courtesy of C. Feng and S. Policastro, NRL.*

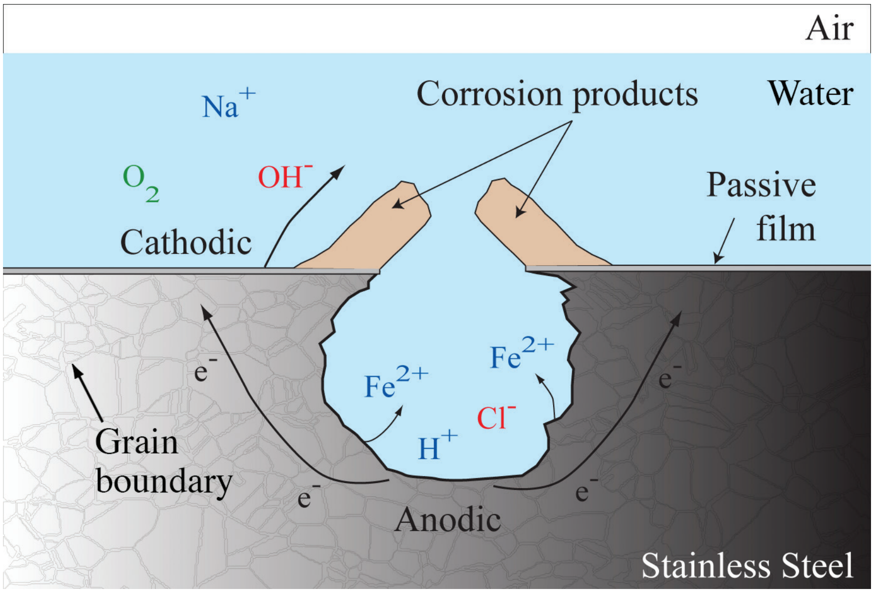


FIGURE 2. Corrosion in metals, such as stainless steel, is the result of electrochemical reactions and mass transport in an electrolyte solution. An irregular corrosion front develops due to the material microstructure.

> "You can use COMSOL Multiphysics with the Corrosion Module to solve this problem. All the work that previously seemed so difficult, now is so easy because you have the module doing a lot of the work for you."

due to microstructure have not been considered. Our goal is to perform fully-coupled multiphysics modeling of pit growth under the application of mechanical forces to quantify the overall effect on structural integrity with material microstructure taken into account."

The irregular corrosion growth due to the metal microstructure is shown schematically in Figure 2 and arises because of the unique size and shape of each individual grain. Each grain can also have a particular crystallographic orientation that can affect the corrosion rate or front movement locally. Secondary phases, precipitates, and twin boundaries are additional features of a metal that can affect the initiation and growth of corrosion pits.

## CORROSION SIMULATIONS WITH METAL MICROSTRUCTURE

"A complete description of pit growth," explains Qidwai, "requires the coupling of electrochemical and mass transport equations for multiple ionic species and constitutive descriptions of reaction rates and species diffusion in the electrolyte, while tracking the metal-electrolyte interface or corrosion front whose movement depends upon the history of the solution." Figure 2 depicts the complex corrosion mechanism simulated by Qidwai in COMSOL Multiphysics® and Figure 3 shows the corresponding model geometry used to evaluate pit growth in metals.

"In developing a complex model, our strategy is to start with simpler numerical studies. Currently in our simulations we solve the electrochemical and mass transport equations separately. In future work, we will create a fully-coupled electrochemical mass transport model of corrosion." To create their models, they have used the transport of diluted species physics for mass transport, the Laplace and Poisson's equations for the electric potential, and the moving mesh (ALE) technology for the corrosion front. "You can use COMSOL Multiphysics with the Corrosion Module to solve this problem," says Qidwai. "All the work that previously seemed so difficult, now is so easy because you have the module doing a lot of the work for you."

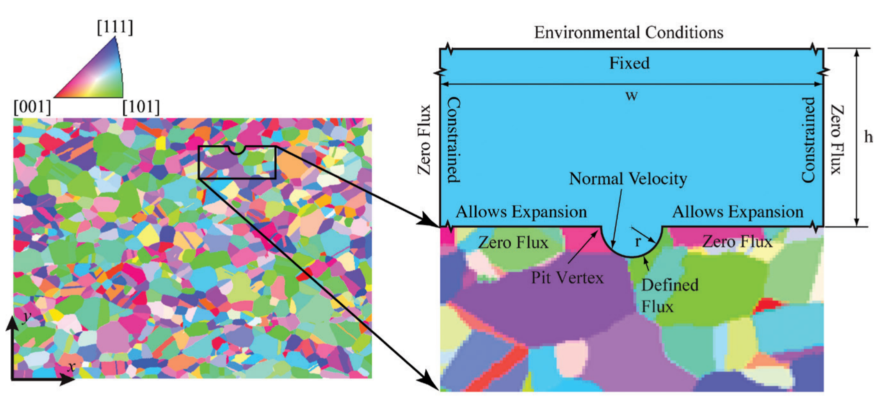


FIGURE 3. At right, the model geometry implemented in COMSOL Multiphysics to evaluate pit growth in metals. The reconstructed metal microstructure, at left, was determined using orientation imaging microscopy at NRL. The colored legend corresponds to the crystallographic orientation of each grain.

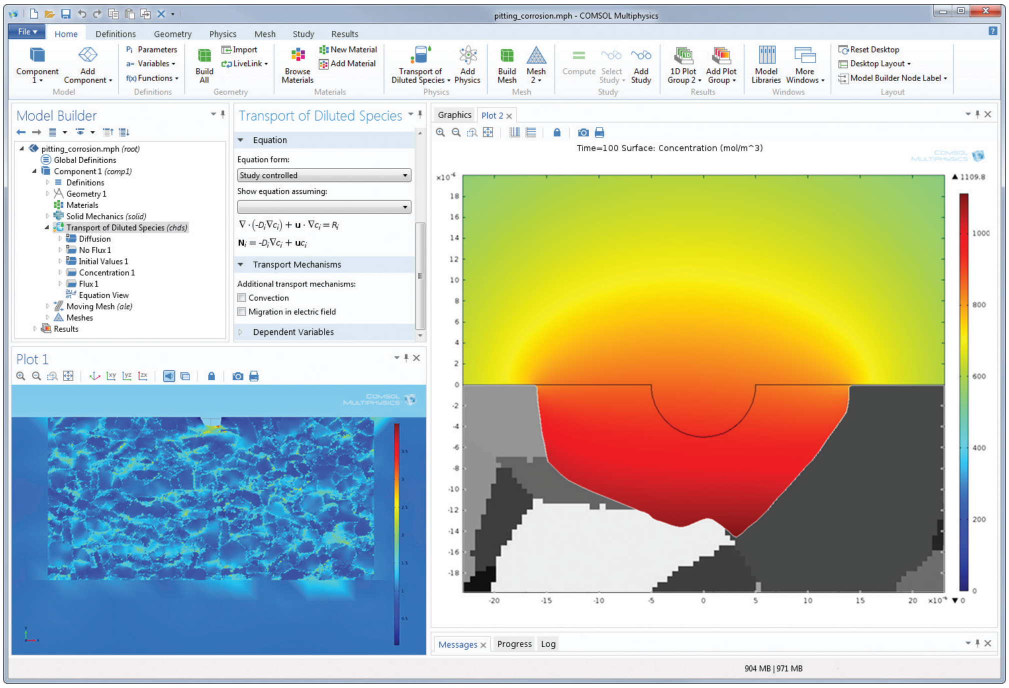


FIGURE 4. Screenshot of the COMSOL environment. Plot 1 shows the von Mises stress in the metal with regions of higher stress surrounding the pit. Plot 2 demonstrates pit growth with an irregular corrosion front and shows the distribution of average metal concentration in the electrolyte.

Incorporating the microstructure into a multiphysics model of pitting corrosion is a formidable challenge tackled initially at NRL through the use of orientation imaging microscopy (OIM) to acquire 3D images of the metal microstructure. An OIM-based reconstructed image of steel is shown in Figure 3.

An integrated method was used to incorporate the microstructure of 316 steel into a multiphysics model of pitting corrosion implemented in the COMSOL environment. “At every location along the corrosion front, we have to determine the crystal orientation to calculate the corresponding pitting potential, which in turn determines the corrosion rate and movement of the front,” says Qidwai. The pitting potential is determined in MATLAB® for a particular crystallographic orientation and ultimately used by the COMSOL model to calculate the corrosion rate and advance the corrosion front. “LiveLink™ *for* MATLAB® has been an essential feature for us in order to include the effect of the metal microstructure.” The properties of 316 steel were custom-defined in the model. Simulation results in the COMSOL environment, presented in Figure 4, demonstrate localized loss of material due to pitting.

In developing their multiphysics model of pitting corrosion, Qidwai found that “COMSOL is so versatile that it will give you a solution even for very complex applications. This is where experimental validation is the key.” Insight gained from their simulations has already provided the impetus for the development of a novel experimental method to evaluate corrosion at the micron scale. The results from the experiments will be used to validate the model and establish the relationship between microstructure, pit shape, and growth.

From left to right: Siddiq Qidwai (NRL), Virginia DeGiorgi (NRL), and Nithyanand Kota (Leidos Corp.) are researching the fundamental mechanism of corrosion in metals.

## THE FUTURE OF CORROSION PREVENTION

As the model is validated and further evolves, it will also include fully-coupled structural mechanics analyses to elucidate the impact of pit growth in a metal on its strength and reliability. At present, a decoupled structural analysis of microstructural steel has been successfully implemented as shown in Figure 4. Qidwai and his team at NRL are also actively developing methods to quantify the relationship between microstructure, pit growth, and mechanical performance. “Establishing this relationship is our ultimate goal and will enable material designers to create materials that better resist and even prevent corrosion, therefore reducing the exorbitant cost and inconvenience shared by everyone.” ■



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