

PRF# 57643-DNI10

**Project Title:** Modeling the collaborative effect of microstructure and corrosion on crack-growth resistance and pattern

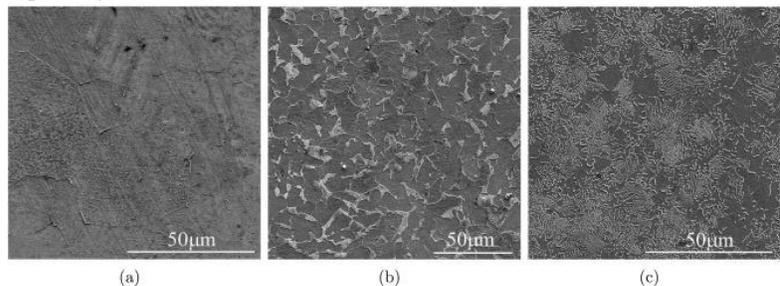
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**Overview:** A material's crack growth resistance depends on its resistance to the creation of new free surfaces, as well as its deformation characteristics, particularly those related to dissipation, which in turn are strongly influenced by the material's microstructure, and the imposed service and loading conditions. In this work we focus on understanding and modeling the collaborative effect of the material's microstructure and environmental assisted degradation on the mechanical response of structural materials. During the first year of this project (09/2017 to 08/2018) we focused on two sub projects. The sub project 1 focused on experimentally characterizing the synergistic effects of localized corrosion, in particular intergranular corrosion, and imposed tensile strain rate on the overall mechanical and electrochemical response of a high strength aluminum alloy, AA7075. In the sub project 2 we focused on modeling the effect of the damage induced by grain boundary diffusion together with the damage induced by solute (oxygen) diffusion along grain boundaries on crack growth under cyclic loading conditions. In the second year of this project (09/2018 to 08/2019) we focused on characterizing and modeling microstructural influence on hydrogen permeation and trapping in pure iron and two ferritic-pearlitic steels, AISI 1018 and AISI 4340. The key outcomes of the project, the overall impact of the project on PI's career, and education and training of students are summarized below.

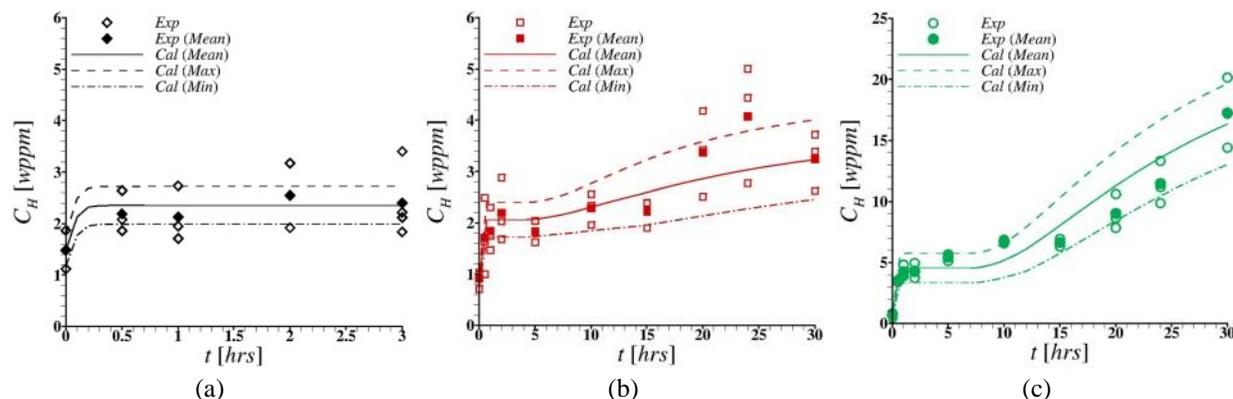
*Microstructural influence on hydrogen permeation and trapping in steels:* The presence of hydrogen in structural metals and alloys, especially steels, has proven to be a problem warranting a significant amount of attention for over a century. In steels the presence of hydrogen severely degrades mechanical properties such as ductility, fracture toughness and fatigue life. The degrading effect of hydrogen on the mechanical properties of structural metals and alloys is commonly referred to as hydrogen embrittlement. The mechanisms of hydrogen ingress in a material depend on the ability of hydrogen to enter and diffuse within the bulk as various lattice imperfections and microstructural features either hinder diffusion or act as trapping sites. The surface of the specimen represents an initial energy well for hydrogen ingress and diffusion in the bulk, while the binding energy of hydrogen with an imperfection or microstructural feature dictates the trapping susceptibility of the hydrogen. The trapping of hydrogen in the bulk of the material has been suggested to reduce the deleterious effect of hydrogen on mechanical properties by reducing the amount of mobile hydrogen in the material. Because the trapped hydrogen must overcome a binding energy larger than that for lattice diffusion before it can be released. This clearly suggests that a quantitative understanding of the role of microstructural features on trapping hydrogen can pave the way to designing material microstructures that drastically reduce the risk of hydrogen embrittlement in structural metals and alloys.

The objective of this work is to quantify the microstructural influence on hydrogen permeation and trapping in pure iron and two ferritic-pearlitic steels, AISI 1018 low-carbon steel and AISI 4340 high strength alloy steel. To this end, the initial microstructure of the three materials are thoroughly characterized and the hydrogen is introduced into cylindrical specimens of these materials through electrochemical charging. The total hydrogen content of the specimens are quantified following gas fusion analysis principle commonly termed as melt extraction. The experimentally measured variation of total hydrogen concentration with electrochemical charging time in the specimens of all three materials are then modeled using a novel modeling framework. The coupled experimental and modeling work allows us to understand and quantify the influence of various defects and microstructural features on hydrogen permeation and trapping.

The representative microstructures of commercially pure iron, AISI 1018 low carbon steel and AISI 4340 alloy steel considered in this work are shown in **Fig. 1**. The microstructure of commercially pure iron is single phase and polycrystalline, while that of 1018 and 4340 steels are dual phase consisting of ferrite grains and pearlitic particles.



**Figure 1:** Representative secondary electron SEM images showing the microstructures of as-received, (a) commercially pure iron, (b) AISI 1018 low carbon steel, and (c) AISI 4340 high strength alloy steel.



**Figure 2:** Comparison of calculated (*Cal*) and experimentally (*Exp*) measured variation of hydrogen concentration,  $C_H$ , with electrochemical charging time,  $t$ , in (a) Pure Iron, (b) AISI 1018 steel and (c) AISI 4340 steel.

The hydrogen was introduced into cylindrical specimens of all three materials through electrochemical charging. The total hydrogen content of the specimens were then quantified following gas fusion analysis principle commonly termed as melt extraction. Furthermore, the experimentally measured variation of hydrogen concentration with electrochemical charging time in the specimens of all three materials were modeled using a modeling framework based on Fickian diffusion equations including the relevant microstructural features, electrochemical charging conditions and three-dimensional geometry of the specimen that affect the overall diffusion behavior. A comparison of experimentally measured variation of hydrogen concentration as a function of electrochemical charging time with the model predictions for all three materials are shown in **Fig. 2**. From **Fig. 2**, a very good correlation between the calculated and the experimental average values of hydrogen concentration is noted. Additionally, most experimental data lie within the plus/minus one standard deviation of the calculated values. In the calculations the variations in hydrogen concentration values for fixed electrochemical charging times is due to variations in the defect/trap densities leading to variations in both the apparent diffusivity and saturation concentration of hydrogen in the traps.

Our results clearly highlight the microstructural influence on hydrogen permeation and trapping. In particular, the results quantitatively show that, (i) unlike pure iron, there are at least two types of hydrogen trapping sites in 1018 and 4340 steels with significantly different permeation activation and binding energies, (ii) the apparent diffusivity of hydrogen in trap 1 (ferrite grain boundaries and dislocations in ferrite) is greater than that in trap 2 (ferrite/cementite interfaces in the pearlitic microstructure), (iii) the difference in the apparent diffusivity of the two traps results in two stage permeation and trapping of hydrogen in both 1018 and 4340 steels with increasing electrochemical charging times, and (iv) the saturation concentration of hydrogen in trap 1 is less than that in trap 2 in both 1018 and 4340 steels. The estimated permeation activation and binding energies for the three materials and microstructural features therein show that the permeation of hydrogen is easy through the ferrite/cementite interfaces in the pearlitic microstructure compared to grain boundaries and dislocations. But the grain boundaries and dislocations act as stronger hydrogen traps than the ferrite/cementite interfaces in the pearlitic microstructure. Also the ease of permeation of hydrogen through coarse pearlitic microstructure is slightly greater than fine pearlitic microstructure. Our results also demonstrate that material and component design against hydrogen embrittlement requires the consideration of the synergistic contribution of permeation as a result of exposure to a certain environment, as well as diffusion within the material or the component. The methodology developed in this work allows for the design of microstructures by simultaneously accounting for both, hydrogen permeation and binding.

**Impact on PI's Career, and Education and training of Students:** This ACS PRF DNI grant has provided the much-needed platform for the PI to venture in the field of chemo-mechanics. So far, the project has yielded three publications in reputed peer-reviewed journals. During the second year of this project three graduate students including two female students were partially supported by this grant. In addition, one female undergraduate student was partially supported as summer intern by this grant. The graduate and undergraduate students involved in this project are trained on chemo-mechanical testing, Electron Microscopy, Electrochemical Impedance Spectroscopy, melt extraction techniques, diffusion modeling, finite element modeling and large-scale parallel computing techniques relevant to modeling material degradation.