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 have 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. The key outcomes of the two sub projects, the overall impact of the project on PI's career, and education and training of students are summarized below.

Sub Project 1, *Synergistic effects of corrosion and slow strain rate loading on the mechanical and electrochemical response of an aluminum alloy:*

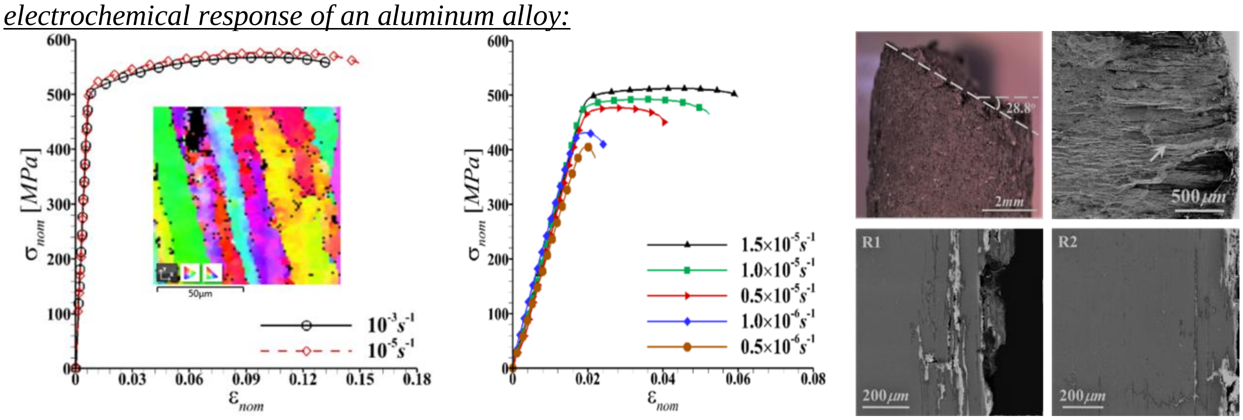

Figure 1: (*Left*) EBSD map of the microstructure of undeformed AA7075 along the axis of the tensile specimen and the nominal stress-strain curves of the specimens tested in air under uniaxial tension at two imposed nominal strain rates. (*Center*) The nominal stress-strain curves of the AA7075 specimens tested in EXCO solution under uniaxial tension at five imposed strain rates. (*Right*) Optical microscope image of the side view, SEM image of the fracture surface, and SEM images of the mechanically polished longitudinal sections of the specimen fractured under uniaxial tension while immersed in the EXCO solution at a strain rate of 10^{-6} per second.

The microstructure of the high strength aluminum alloys, such as AA7075, contains intermetallic particles to enhance the mechanical properties of the material. But these intermetallic particles can adversely affect the formation of the natural passive layer, and can result in the formation of micron-scale galvanic cells resulting in localized corrosion. It is also generally recognized that the processes of localized corrosion are aggravated by the presence of tensile stresses. Following this, the objective of this work was to characterize the synergistic effects of localized corrosion and imposed tensile strain on the overall mechanical and electrochemical response of the material. To this end, tensile specimens of AA7075 with grains aligned parallel to the tensile axis were subjected to a range of slow strain rate tensile loading while immersed in the EXCO solution, **Fig. 1**. The degradation in the mechanical response of the material was measured and the emerging electrochemical characteristics of the electrolyte/specimen interface using electrochemical impedance spectroscopy (EIS) were characterized for a range of imposed strain rates. The EIS measurements coupled with the post-mortem microscopic characterization of the specimens rationalized the effects of corrosion and the imposed strain rate on the degradation in the mechanical response of the material. The overall failure mechanism that emerges is such that the exposure of the specimen to the corrosive environment results in both uniform and localized (intergranular) corrosion of the specimen. The imposed tensile strain on the specimen results in breakdown of the passivating film preferentially along the grain boundaries. Furthermore, the continued tensile straining of the specimen results in preferential cracking of the corroded transverse grain boundaries thus biasing the corrosion pathway in the transverse direction. The interplay of preferential corrosion and the tensile straining eventually results in the formation of a circumferential crack of critical crack length and final fracture of the specimen.

Sub Project 2, *Environmentally enhanced creep crack growth by grain boundary cavitation under cyclic loading:*

In this project we carried out plane strain finite element calculations of mode I crack growth under time varying imposed stress intensity factor. The finite element calculations were based on a constitutive relation that couples creep deformation and damage due to grain boundary cavitation including the embrittling effect of solute (oxygen) diffusion along grain boundaries. Isothermal analyses were carried out for two sets of material and grain boundary parameters: (i) parameter values representative of HASTELLOY® X; and (ii) parameter values representative of P91. The detrimental effect of environmentally assisted grain boundary embrittlement on HASTELLOY® X is highlighted in **Fig. 2**. The variation of the predicted cyclic crack growth rate with imposed stress intensity factor range was found to be in good quantitative agreement with experimental results in the literature for both HASTELLOY® X and P91. Paris law behavior, i.e. the cyclic crack growth rate depending on the imposed stress intensity factor range raised to a power, emerges naturally in the calculations. Parametric studies show that the cyclic crack growth rate and the Paris law exponent are more sensitive to variations in the grain boundary diffusivity, the solute diffusivity and a parameter characterizing the environmental embrittling effect than to parameters characterizing the creep response of the material.

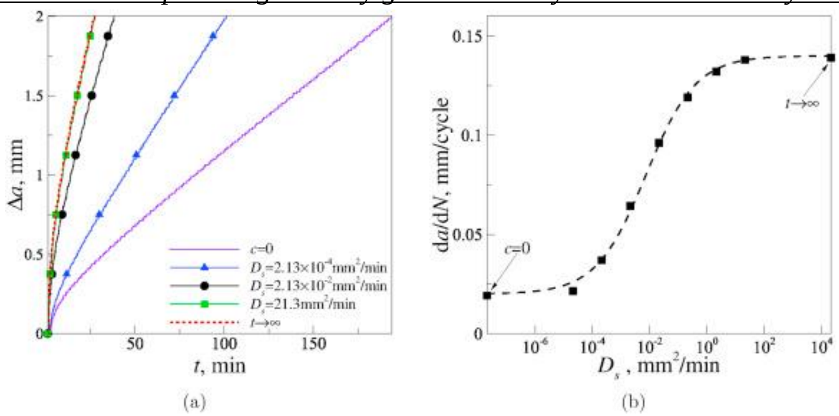

Figure 2: The effect of the solute diffusivity, D_s, on cyclic crack growth. Material parameters representative of HASTELLOY® X at 1200K are used in the calculations. (a) Curves of crack extension, Δa, versus time, t. (b) The dependence of the cyclic crack growth rate, da/dN, on D_s. The values of with no grain boundary solute weakening, $c = 0$, and for the solute (oxygen) concentration corresponding to $t\rightarrow\infty$ are also shown.

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 one publication and a second paper has been submitted for publication to a reputed peer-reviewed journal. During the first year of this project one female graduate student was fully supported by this grant, and two female graduate students were partially supported. In addition, one female undergraduate student was supported for four weeks as summer intern by this grant. The graduate and undergraduate students involved in this project are trained on slow strain rate stress corrosion cracking tests, Electron Microscopy, Electrochemical Impedance Spectroscopy, and large-scale parallel computing techniques relevant to corrosion and fracture modeling.