A Generalized Entropic Framework of Damage: Theory and Applications to Corrosion-Fatigue

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5. Prof. C. Wang (Corrosion/electrolysis consultant)
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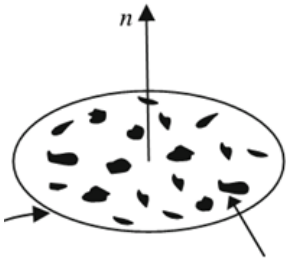
Objectives

- Description of degradation mechanisms and resulting damages within the irreversible thermodynamics framework
- Improved understanding of the coupled mechanisms
- Development of an entropic corrosion-fatigue damage model
- Confirmatory testing of the corrosion-fatigue model
- Investigation of applications to structural integrity and reliability assessment
- Search for applications to Prognosis and Health Management (PHM) of structures

Motivation

- Common definitions of damage are based on observable markers of damage which vary at different geometries and scales

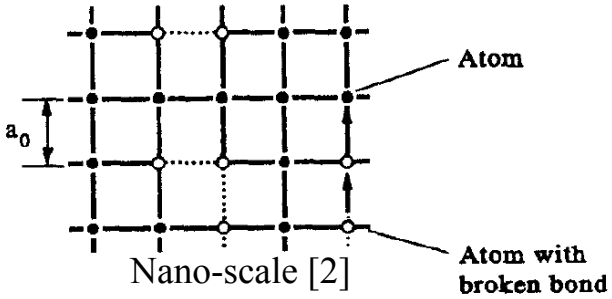
  - At the macroscopic level: Observable markers of damage (e.g. crack size, pit densities, weight loss)
  - Macroscopic fatigues markers include: reduction of elasticity modulus, variation of hardness, cumulative number of cycle ratio, reduction of load carrying capacity, crack length and energy dissipation
  - When markers of damage observed in real structures 80%-90% of life has been expended



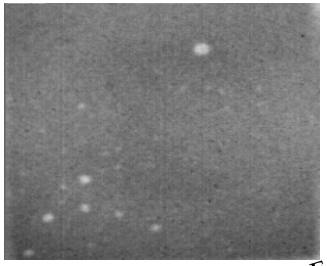
Micro-scale:

$$D(\boldsymbol{n}) = \frac{A_0 - A_e}{A_0}$$

Continuum damage mechanics [1]



Nano-scale [2]



Meso-scale

Entropy and Damage

- Entropy provides a unified and broad measure of damage in terms of energy dissipations of multiple irreversible degradation processes
- Entropy enables us to model multiple competing degradation processes contributing to damage
- Entropy is independent of the path to failure for a system ending at similar total entropy at the time of failure
- Entropy accounts for synergistic effects arising from interactions between multiple degradation processes
- Entropy applies to all scales

Damage and Entropy

Degradation mechanisms → Damage → Dissipation energies → Entropy generation

$$\text{Damage} \equiv \text{Entropy}$$

An entropic theory follows:

Failure occurs when the total entropy exceeds the entropic-endurance of the system

- Entropic-Endurance is the capacity of the system to withstand entropy
- Entropic-Endurance of the same systems are equal
- Entropic-Endurance of different systems are different
- Entropic-Endurance is measurable and involves stochastic uncertainties

Total Entropy

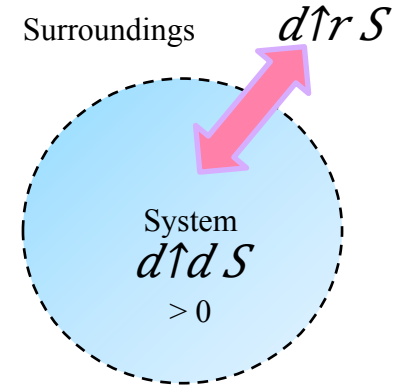
- The variation of *total entropy*, dS, is in the form of: $dS = d_r S + d_d S$.

  $d_r S$ = exchange part of the entropy supplied to the system by its surroundings through transfer of matters and heat: $d_r S/dt = -\int_\Omega \mathbf{J}_s \cdot \mathbf{n}_s \, dA$

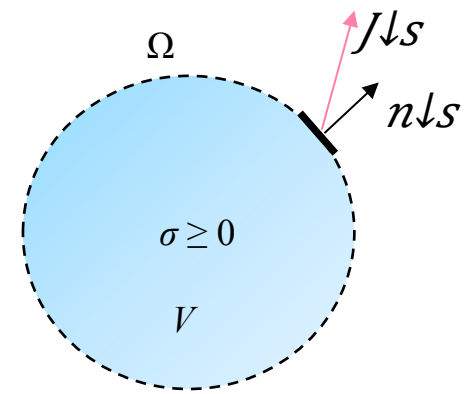
  $d_d S$ = irreversible part of the entropy produced inside of the system: $d_d S/dt = \int_V \sigma dV$.

- Divergence theorem leads to: $ds/dt + \nabla \cdot \mathbf{J}_s = \sigma$, where, s is the specific entropy per unit mass.

- The evolution trend of the damage, D, according to our theory is dominated by the entropy generated: $D|_t \sim \int_0^t [\sigma|X_i(u), \mathbf{J}_i(u)] du$



$dS = d_r S + d_d S$



J=entropy flux; σ=entropy generation/unit volume/unit time

* Imanian, A. and Modarres, M., *A Thermodynamic Entropy Based Approach to Prognosis and Health Management*, The Annual Conference of the PHM Society, 2014.

Total Entropy Generated (Cont.)

- Entropy generation σ involves a thermodynamic force, X_i, and an entropy flux, J_i as:

$$\sigma = \Sigma_{i,j} X_i J_i (X_j) \; ; \quad (i, j=1, \ldots, n)$$

Note that when synergy between multiple dissipation / damage processes exist Onsagar reciprocal relations define forces and fluxes. For example for Fatigue (f) and Corrosion (c)

$$J_c = L_{cc} X_c + L_{fc} X_f \;\; and \;\; J_f = L_{cf} X_c + L_{ff} X_f$$

- Entr Thermal energy Diffusion energy s Plastic deformation energy ng to damage:

$$\sigma = 1/T^2 \; J_q . \nabla T - \Sigma_{k=1}^{n} J_k (\nabla \mu_k / T) + 1/T \; \tau : \epsilon_p + 1/T$$

Chemical reaction energy External fields energy

$$\Sigma_{j=1}^{r} v_j \; A_j + 1/T \; \Sigma_{m=1}^{n} \; J_m (-\nabla \varphi)$$

J_n $(n=q,k,$ *and* $m)=$ thermodynamic fluxes due to heat conduction, diffusion and external fields, T=temperature, μ_k =chemical potential, v_i =chemical reaction rate, τ=stress tensor, ϵ_p =the plastic strain rate, A_j= the chemical affinity or chemical reaction potential difference, φ= potential of the external field, and L_m= coupling constant.* **

Examples of Force and Flux of Dissipative Processes

- $\sigma = \Sigma_{i,j} X_i J_i (X_j)$; $(i, j=1, \ldots, n)$

Primary process	Thermodynamic force, X	Thermodynamic flow, J	Degradation / Failure Mechanism
Plastic deformation	Stress, σ/T	Plastic strain,	Fatigue, creep, wear
Chemical reaction	Reaction affinity, A_k/T	Reaction rate, v_k	Corrosion, wear
Mass diffusion	Chemical potential,	Diffusion flux, J_k	Wear, creep
Electrochemical reaction	Electrochemical potential,	Current density, i_{corr}/z	Corrosion
Irradiation	Particle flux density, A_r/T	Velocity of target atoms after collision,	Irradiation damage
Annihilation of lattice sites	Creep driving force	Creep deformation rate, R	Creep

Table From: Amiri, M. and Modarres, M., *An Entropy-Based Damage Characterization*, Entropy, 16, 2014.

Entropic-Based Damage from Corrosion-Fatigue (CF)

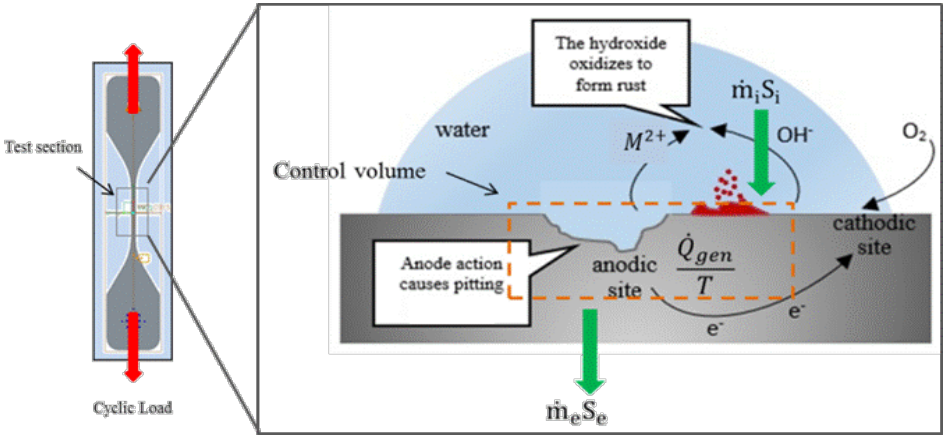
- Oxidation and reduction reactions of metallic electrode, M, under CF:

$$M \leftrightarrow \mathrm{M}\uparrow z\downarrow \mathrm{M}\uparrow + \ +z\downarrow \mathrm{M}\ e\uparrow -$$

$$O + z\downarrow O\ e\uparrow - \ \leftrightarrow R$$

O = Certain oxidant in solution resulting in formation of the reduction product R.

- The entropy production results from:
  - Entropy flow to the surrounding
  - The dissipative processes:
    - Corrosion reaction processes
    - Electrochemical processes
    - Mechanical losses
    - Diffusion losses
    - Hydrogen embrittlement losses



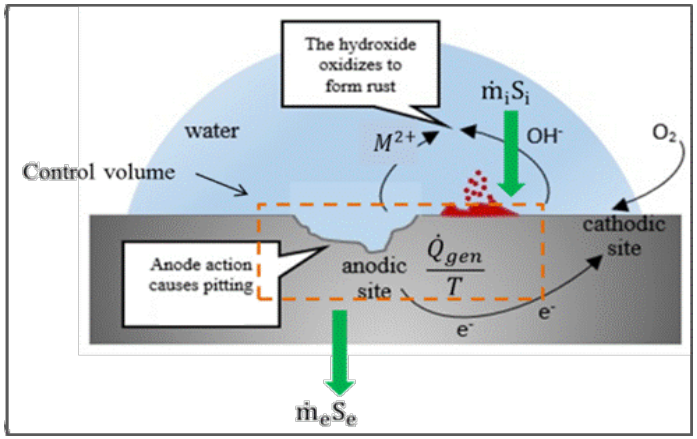
Entropy Exchange in CF

- The amount of entropy exchanged in CF:

$$d_{r}s/dt = \sum_{i} \dot{m}_{i} s_{i} - \sum_{e} \dot{m}_{e} s_{e} + \sum_{j} \dot{Q}_{gen}/T_{j}$$

$\dot{m}_{i} s_{i}$ and $\dot{m}_{e} s_{e}$ = entropy flows entering and exiting the control volume.

- In corrosion the rate of corroded mass obeys $\dot{m} = \dot{m}_{i} = \dot{m}_{e}$.



Entropy Generation in CF

- Contribution from corrosion activation over-potential, diffusion over-potential, corrosion reaction chemical potential, plastic and elastic deformation and hydrogen embrittlement to the rate of entropy generation [1]:

Electrochemical dissipations

$$\sigma = 1/T\,(J_{M,a}\, z_M\, F E_{M,act,a} + J_{M,c}\, z_M\, F E_{M,act,c} + J_{O,a}\, z_O\, F E_{O,act,a} + J_{O,c}\, z_O\, F E_{O,act,c})$$

Diffusion dissipations

$$+1/T\,(J_{M,c}\, z_M\, F E_{M,conc,c} + z_O\, F J_{O,c}\, E_{O,conc,c})$$

Chemical reaction dissipations

$$+1/T\,(J_{M,a}\, \alpha_M\, A_M + J_{M,c}\,(1-\alpha_M)\, A_M + J_{O,a}\, \alpha_C$$

Mechanical dissipations

$$J_{M,a}\,(1-\alpha_C)$$

Hydrogen embrittlement dissipation

$$+1/T\, \epsilon_p : \tau + 1/$$

$$+\sigma_H$$

T = temperature, z_M = number of moles of electrons exchanged in the oxidation process, F = Farady number, $J_{M,a}$ and $J_{M,c}$ = irreversible anodic and cathodic activation currents for oxidation reaction, $J_{O,a}$ and $J_{O,c}$ = anodic and cathodic activation currents for reduction reaction, $E_{M,act,a}$ and $E_{M,act,c}$ = anodic and cathodic over-potentials for oxidation reaction, $E_{O,act,a}$ and $E_{O,act,c}$ = anodic and cathodic over-potentials for

CF Simplifying Assumptions

1. Entropy flow due to mass transfer and heat exchange negligible
2. Diffusion losses are eliminated assuming well mixed solution
3. Effect of diffusivity and concentration of hydrogen at the crack surface excluded for Aluminum alloys under cyclic loading in the sodium chloride solution (Mason confirms that in fatigue loading > 0.001 Hz less time for diffusion and accumulated hydrogen exists)
4. The Ohmic over-potential effect was minimal by placement of the Luggin capillary close to the working electrode
5. Activation over-potential considered to be result of Mechano-chemical effect.

Corrosion current-potential hysteresis

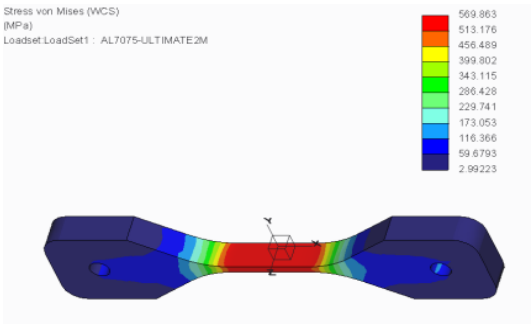
$$\sigma = 1/T\,(\boldsymbol{J}_{M,a}\,\alpha_M A_M + \boldsymbol{J}_{M,c}\,(1-\alpha_M)A_M + \boldsymbol{J}_{O,a}\,\alpha_O A_O + \boldsymbol{J}_{O,c}\,(1-\alpha_O)A_O) + (1/T\,\boldsymbol{\epsilon}_p : \boldsymbol{\tau} + 1/T\,Y\boldsymbol{D})$$

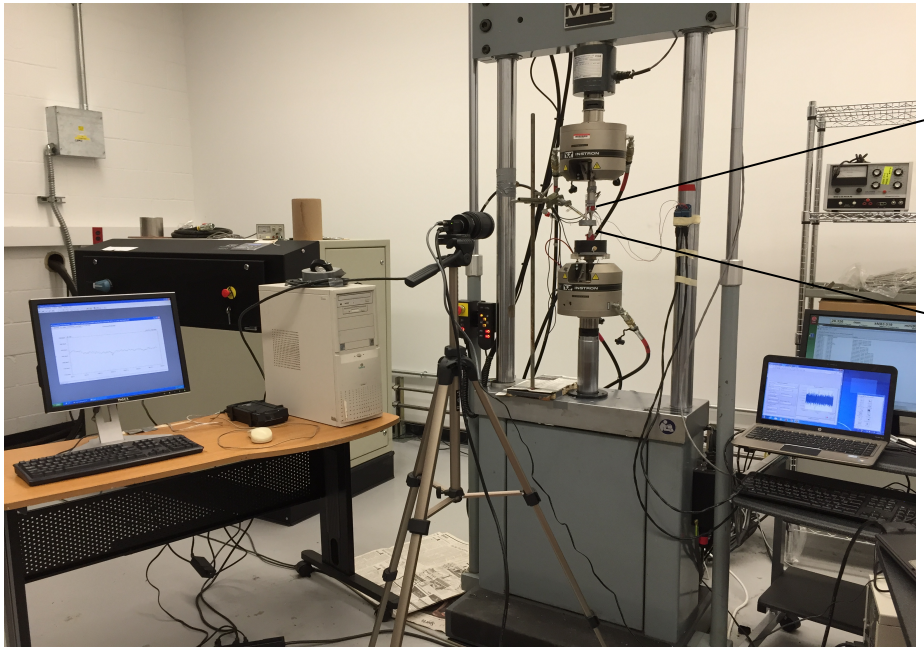
Mechanical hysteresis

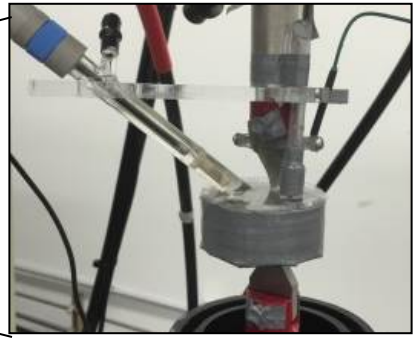
$A = \Sigma_i \nu_i \mu_i$ is mechano-chemical affinity induced by mechano-chemical potential $\mu_i = \mu_i + z_i F(E - E_{corr})$.

Corrosion Fatigue Experimental Set up

- Fatigue tests of Al 7075-T651 in 3.5% wt. NaCl aqueous solution acidified with a 1 molar solution of HCl, with the pH of about 3.5, under axial load controlled and free corrosion potential
- Specimen electrochemically monitored via a Gamry potentiostat using Ag/AgCl reference electrode maintained at a constant distance (2 mm) from the specimen, a platinum counter electrode, and the specimen as the working electrode
- Digital image correlation (DIC) technique used to measure strain

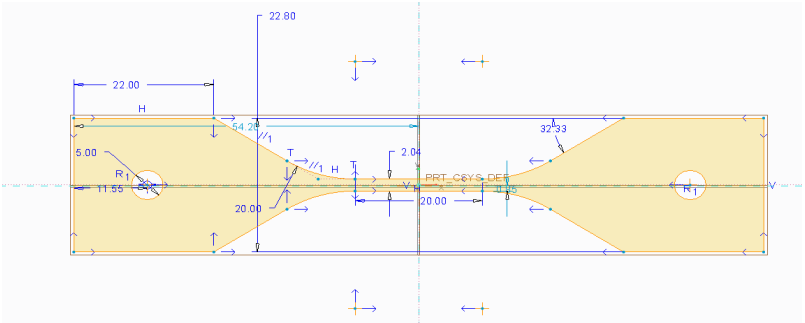


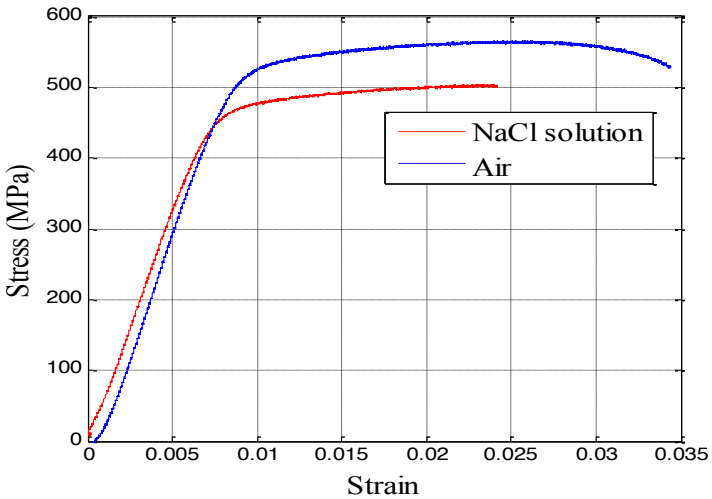




Electrochemical corrosion cell made of plexiglass

CF Test Procedures





First we need to develop $J_i(X_j)$

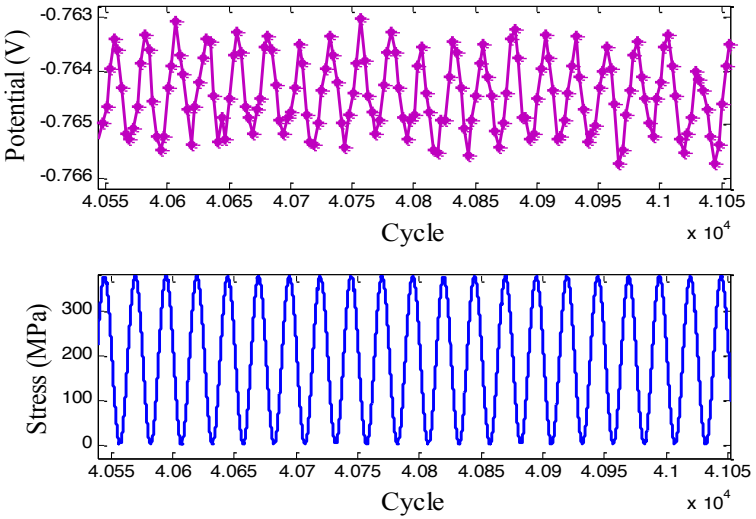
- Performed tensile mechanical test to obtain mechanical and electrochemical properties of the specimen immersed in the corrosive environment

Next the forces and fluxes were measured under CF

- Performed CF tests for 16 samples at 87%, 80%, 70% and 57% of yield stress (460 MPa), load ratio = 0.01, loading frequency=0.04Hz
- Tests stopped after failure of specimens

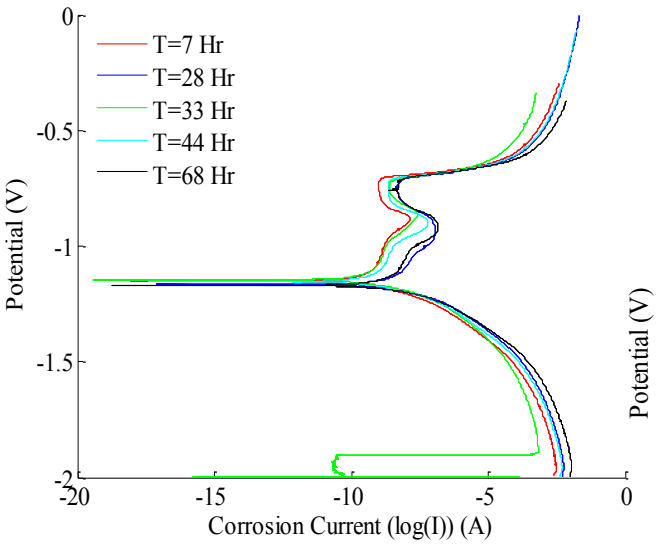
CF Test Procedure- Mechano-Chemical Effect

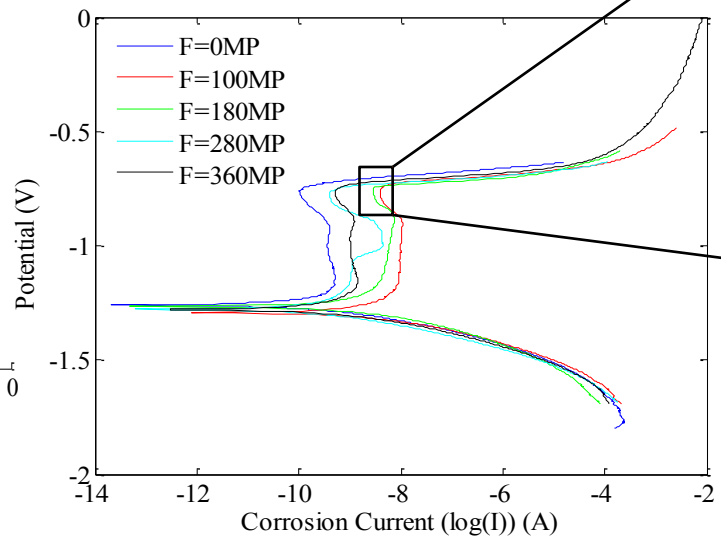
- CF tests done while measuring the open circuit potential (OCP) vs. unstrained reference electrode during load-unload
- In a mechano-chemical effect in CF, an enhanced anodic dissolution flux is induced by the dynamic surface deformation
- Anodic current at the electrode surface, decrease near-surface work hardening, and increase the mobility of dislocation, and hence stimulate fatigue damage
- All showing the Onsager effect discussed earlier

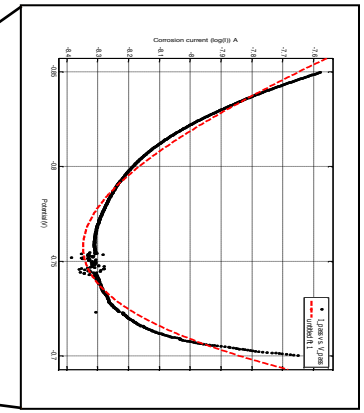


Corrosion Current vs. Potential: Effect of Time and Stress

- To obtain the correlation between *corrosion current and potential*, polarization curves were developed at different stress and immersion values
- Stress and immersion time variations showed stochastic effect on polarization curve
- The sum of the exponential terms showed a good fit to the part of polarization which involved the open circuit potential (OCP)





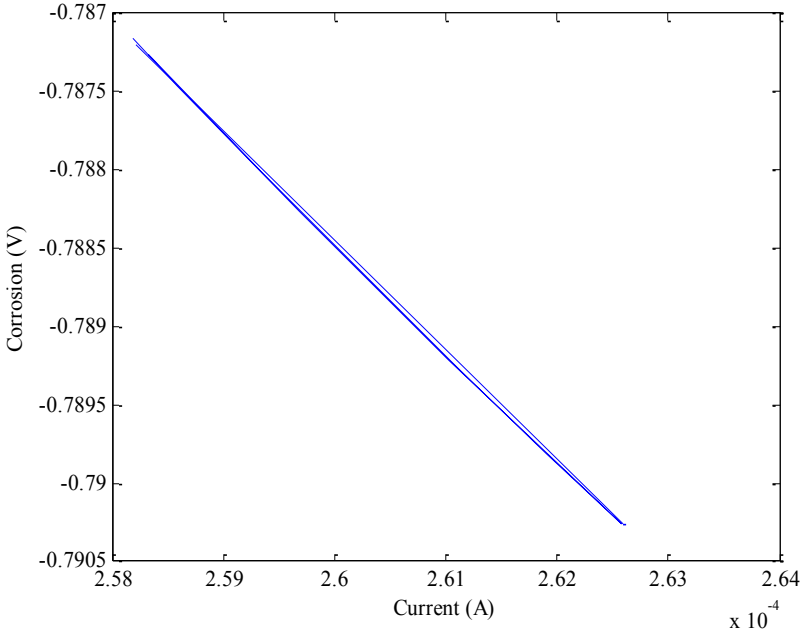


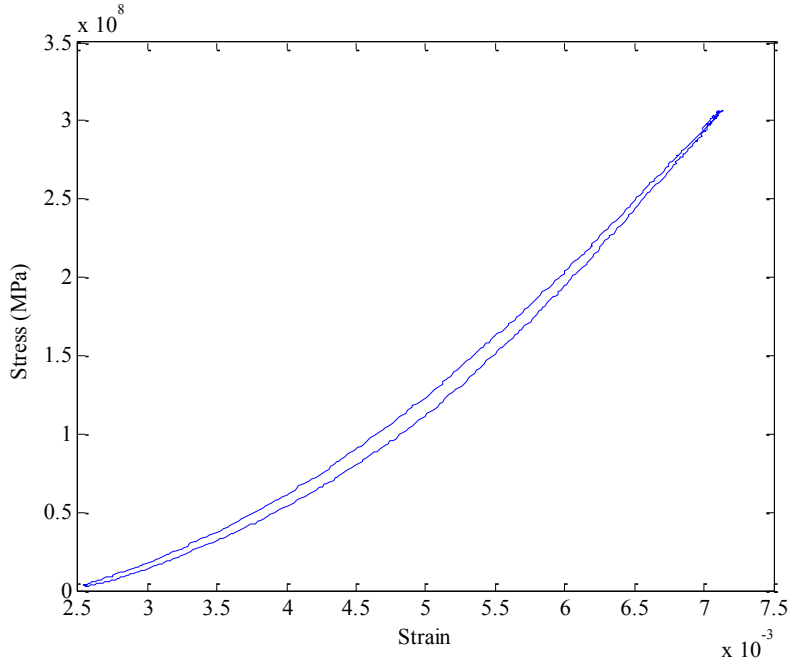
$I = \exp(\alpha V) + \exp(\beta V$

i.e., $J \downarrow i\,(X \downarrow j)$

Entropy Generation in CF

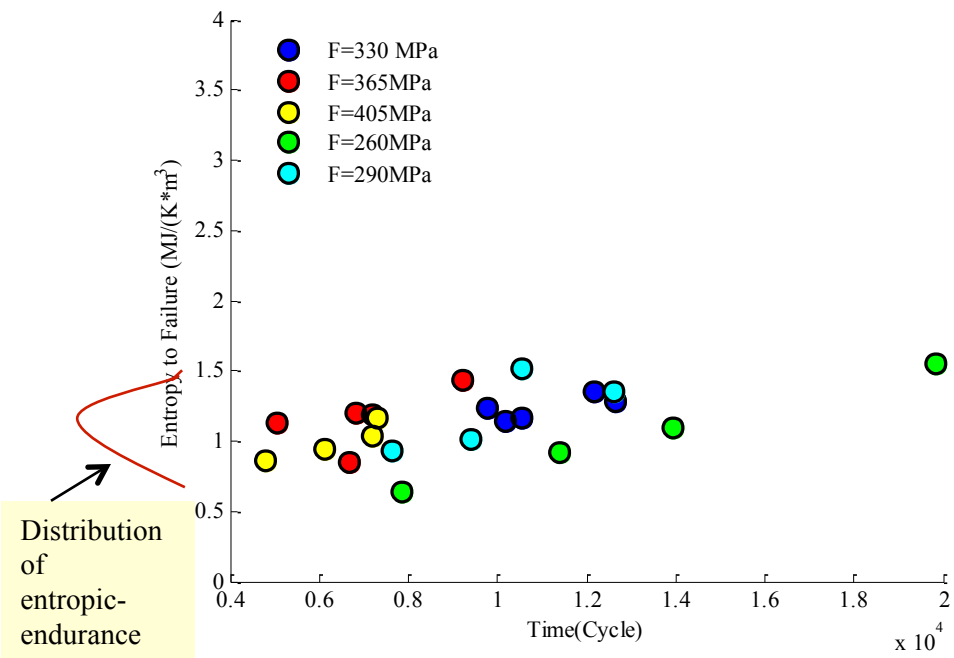
- Total entropy is measured from the hysteresis loops resulted from fatigue (stress-strain) and corrosion (potential-electrical) in each loading cycle

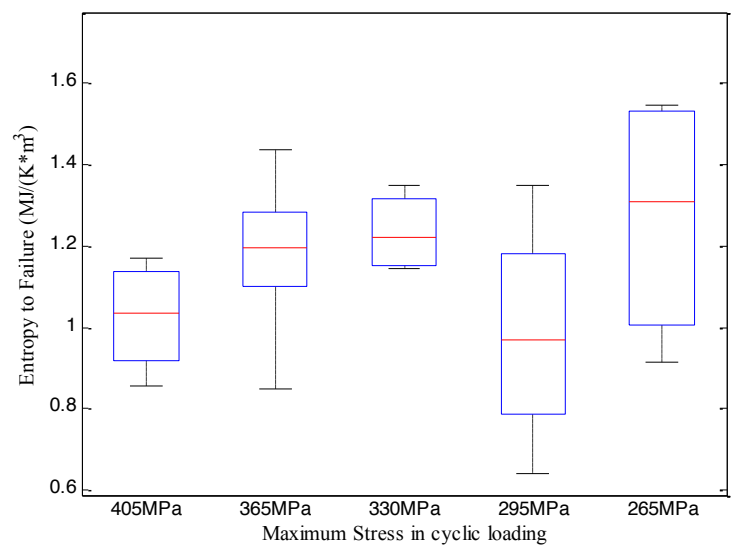




Entropic Endurance and Entropy-to-Failure

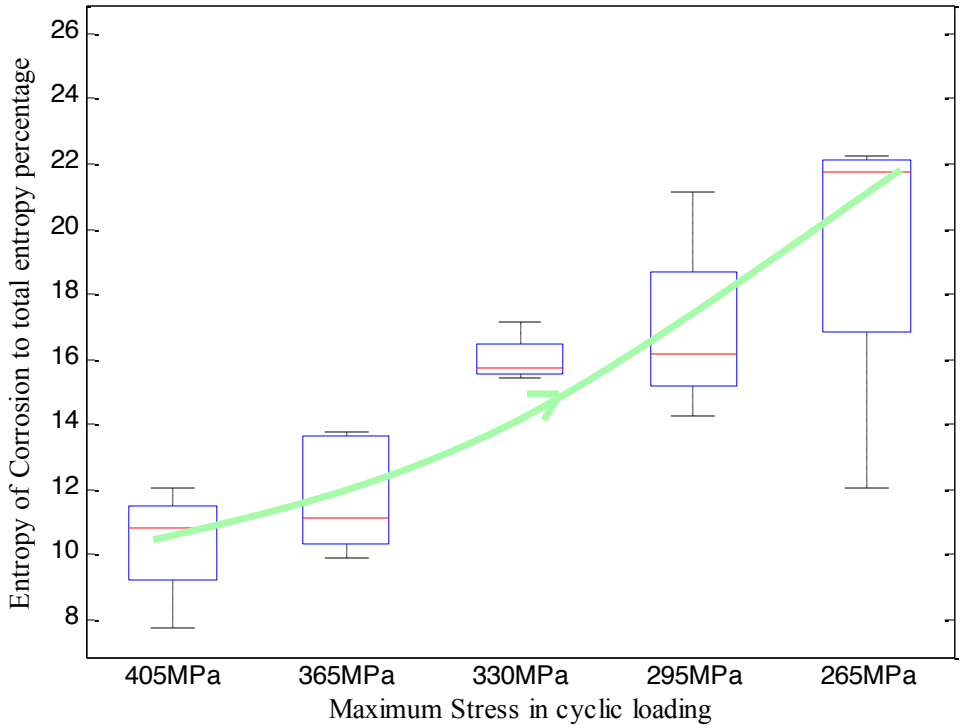
- Similarity of the total entropy at the time of failure supports the proposition of the entropic theory of damage offered in this research
- More tests needed to reduce the epistemic uncertainties and further confirm the theory





Ratio of Corrosion Entropy to the Total Entropy

- Reducing maximum stress allows more time for corrosion thus increasing contribution of corrosion to total entropy
- See ratio of entropy from corrosion to the total entropy versus maximum stress

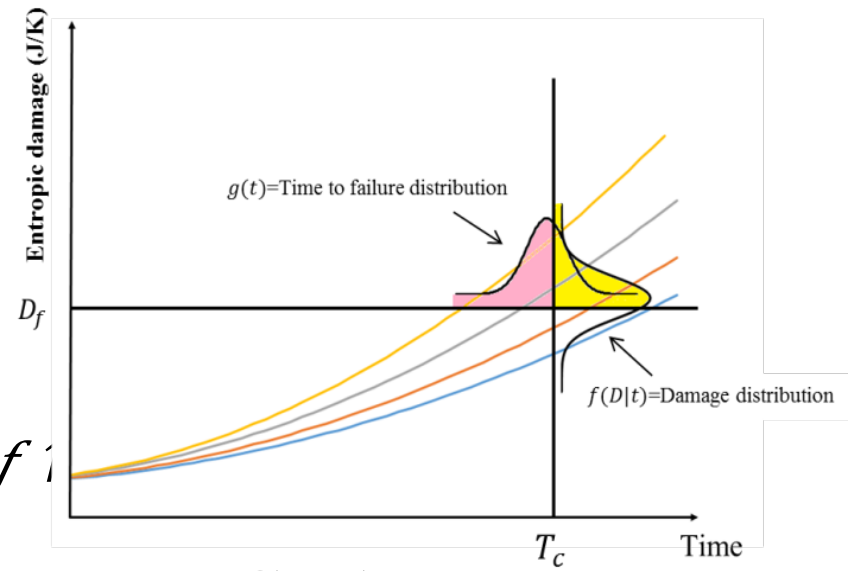


Thermodynamics as the Science of Integrity and Reliability

- Materials, environmental, operational and other types of variabilities in degradation forces impose uncertainties on the total entropy / cumulative damage, D

- Assuming a constant *entropic-endurance*, D_f

- The reliability function can be expressed as [1]



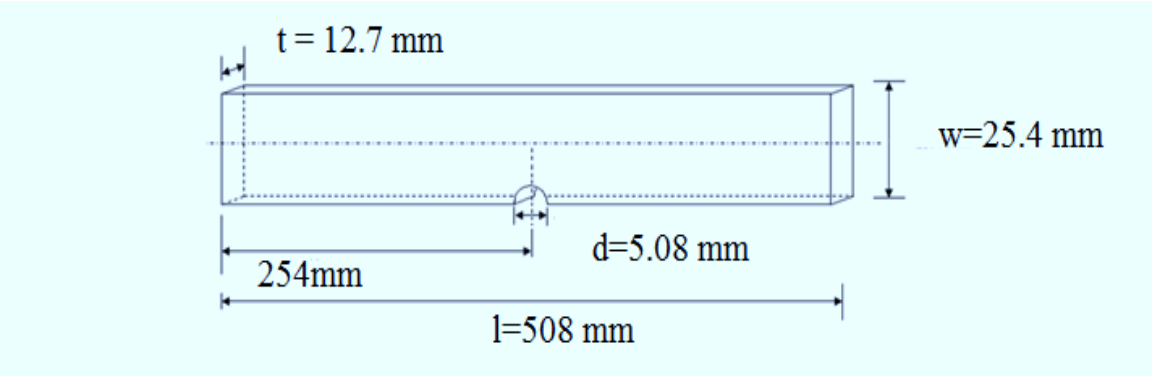
$$R(T_c) = \int_{T_c}^{\infty} g(t)\,dt = 1 - \int_{D_f}^{\infty} f(D|t)\,dD$$

T_c =Current operating time; $g(t)$=distribution of time-to-failure, $f(D|t)$ = distribution of damage at t

[1] A. Imanian. & M. Modarres, *"A Science-Based Theory of Reliability Founded on Thermodynamic Entropy, " Probabilistic Safety Assessment and Management Conference* Honolulu, Hawaii, USA, 2014.

Entropic Characterization of Fatigue-Induced Crack Initiation

- Developed entropy generation terms and physical measures
- Performed Fatigue tests (peak 248 MPa with load ratio of 0.1 and frequency of 2Hz) on Al 7075-T6 notched specimens
- Test stopped when, a small crack detected at the notch

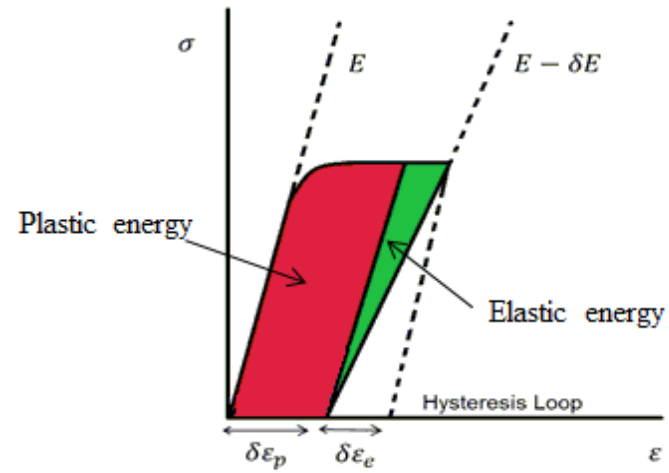


Entropy Generation in Fatigue Damage

- Entropy generation during fatigue:

$$\sigma = \boldsymbol{\tau} : \boldsymbol{\epsilon}_p / T + 1/T\, ZD + 1/T^2\, \boldsymbol{J}_q \cdot \nabla T$$

Plastic energy loss | Elastic energy loss | Heat loss



- For high-cycle fatigue heat conduction term is comparatively negligible

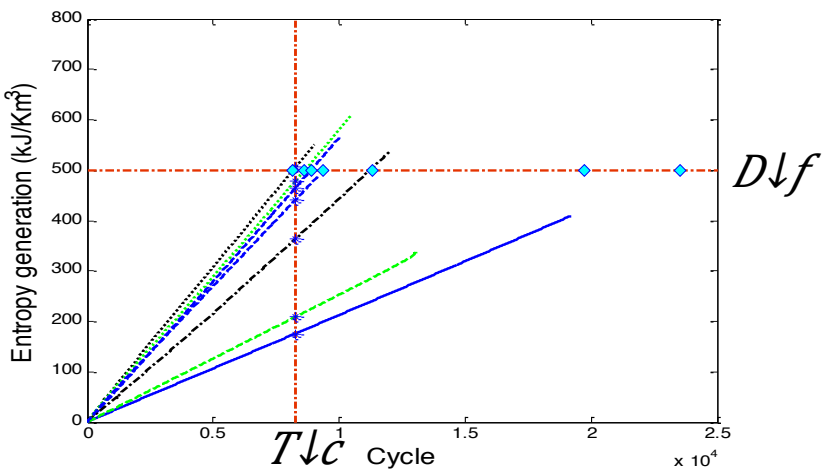
Reliability and Integrity Analysis

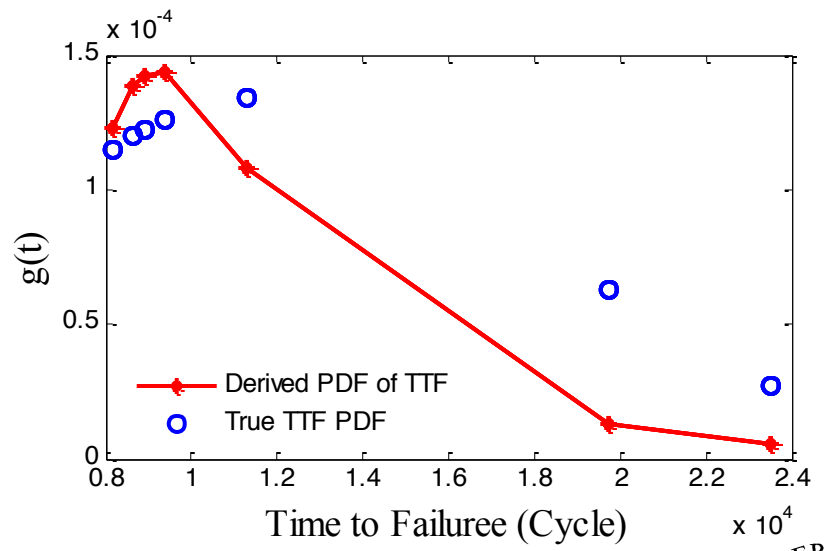
$$F(t)=\int_0^{T_c} g(t)\,dt = 1-\int_0^{D_f} f(D)\,dD$$

Assuming constant entropic damage with slops a_i and transforming variable t with $D_f T_c/D$ by knowing:

$$\begin{cases} a_i t = D_f \\ a_i T_c = D \end{cases}$$

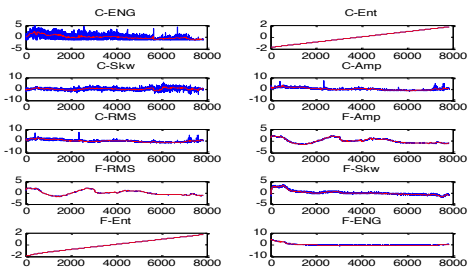
$$g(t)=D_f T_c/t^2 \; f(D_f T_c/t)$$

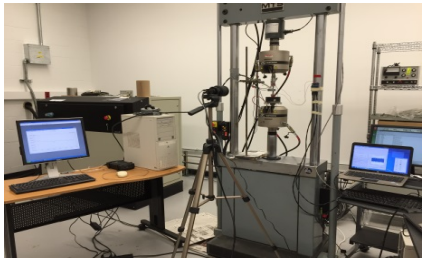




Application of the Entropic PHM Framework

- Proposed PHM framework has been used to predict the RUL of Al samples.





Features:
- Strain RMS
- Strain max amplitude
- Strain skewness
- Mechanical entropy
- Mechanical hysteresis energy
- Potential RMS
- Potential max amplitude
- Potential skewness
- Potential Entropy
- Potential hysteresis energy

Off-Line Modeling

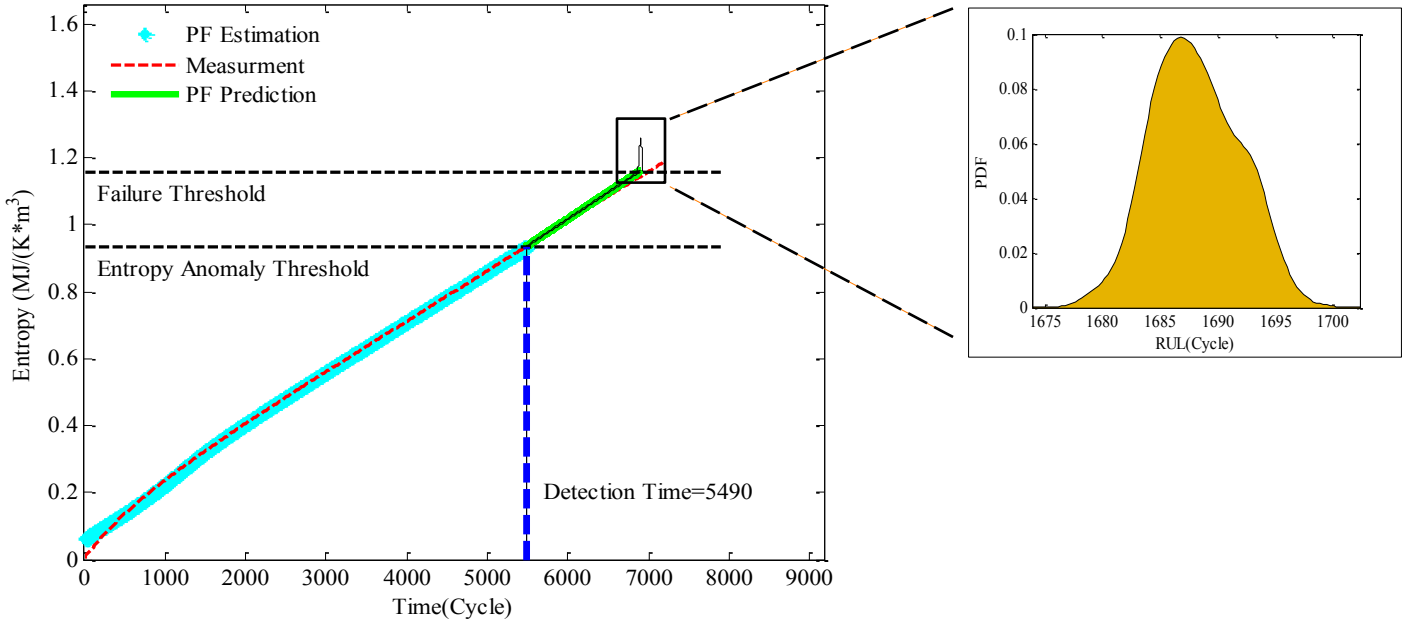
Signal Processing → Feature Extraction → Training Data Classification by the *kNN* Approach

On-Line Health Assessment and Prediction

Dissipative Processes Identification → Entropy Evaluation → Health Assessment and Anomaly Detection → RUL Estimation

An Example of RUL Prediction

- *kNN* is a non-parametric classification method
- Fault level (FL) determined from the output of the *kNN* classification
- An anomaly was acknowledged from FL



Prognastics Results

- By choosing the entropy data as a precursor, *Particle Filter* prediction method helps estimating the RUL
- The difference between mean of estimated RULs and actual RULs showing the efficiency of the entropic-based PHM for structural integrity assessment

Maximum Stress (MPa)	Estimated RUL(%)	Actual RUL(%)
330	17.8	26.4
330	30.3	30.8
330	8.1	23.2
365	11.7	11.0
365	20.2	23.4
405	37.1	32.8
405	28.3	32.8
295	42.6	31.6
295	10.1	29.2
260	43.5	28.9
260	26.3	33.9

Ongoing Activities

- More experiments using varied corrosion medium and slower fatigue
- Modeling and simulating the mechanistic damage evolution in the corrosion fatigue mechanism using the multi-physics tools (COMSOL).
- Comparison of the experimental and simulation results.

Conclusions

- A thermodynamic theory of damage proposed and tested
- Applications to reliability and structural integrity assessments explored
- The proposed theory offered a consistent and science-based model of damage and allowed for the incorporation of all underlying dissipative processes
- Entropy generation function derived and evaluated for corrosion-fatigue degradation mechanism in terms of leading dissipative processes
- Entropic corrosion-fatigue degradation model experimentally studied and supported the proposed theory
- Proposed a PHM framework based on entropic damage

Publications

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Thank you