Thermodynamics of Damage: A Reliability Engineering Perspective

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Acknowledgments

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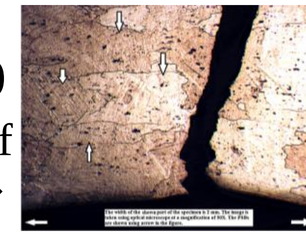
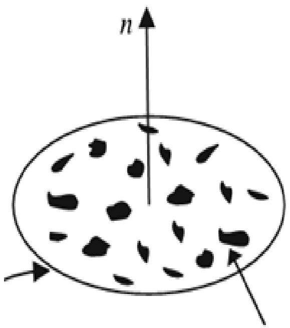
Objectives

- Describe damage resulted from failure mechanisms within the irreversible thermodynamics framework
- Improve understanding of the coupled failure mechanisms
- Develop an example: entropic corrosion-fatigue damage model including confirmatory tests
- Define reliability in the context of the 2^{nd} law of thermodynamics
- Extend the framework to statistical mechanics and information theory definitions of entropy
- 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
  - ➢ Macroscopic Markers of Damage (e.g. crack size, pit densities, weight loss)
  - ➢ Example: Macroscopic Fatigues Markers include: crack length, reduction of modulus, reduction of load carrying capacity
  - ➢ Issue: When markers of damage observed 80%-90% of life has been expended

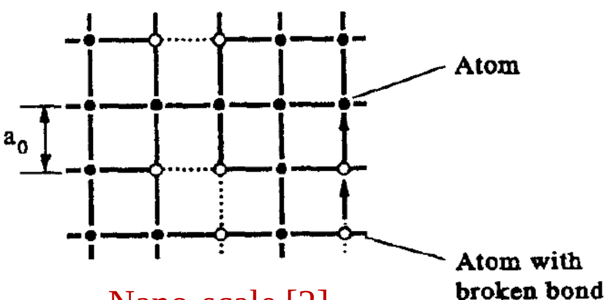




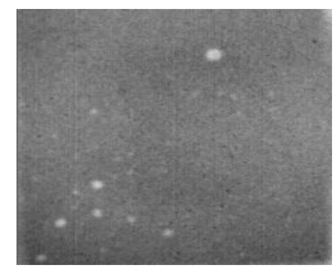
$$D(\boldsymbol{n}) = \frac{A_0 - A_e}{A_0}$$

Continuum damage mechanics [1]

Micro-scale



Nano-scale [2]

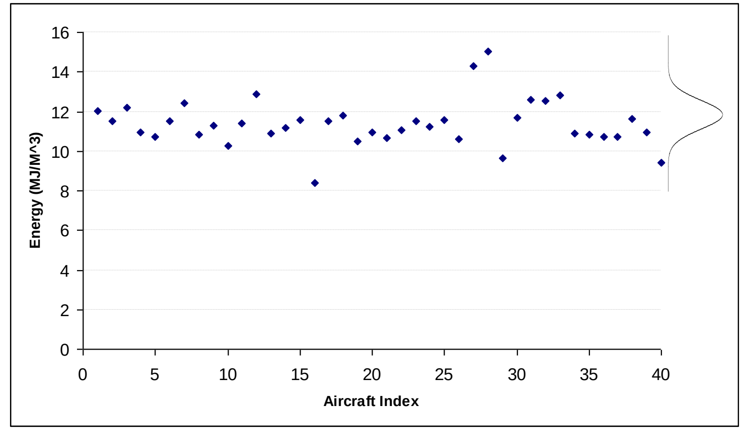


Meso-scale

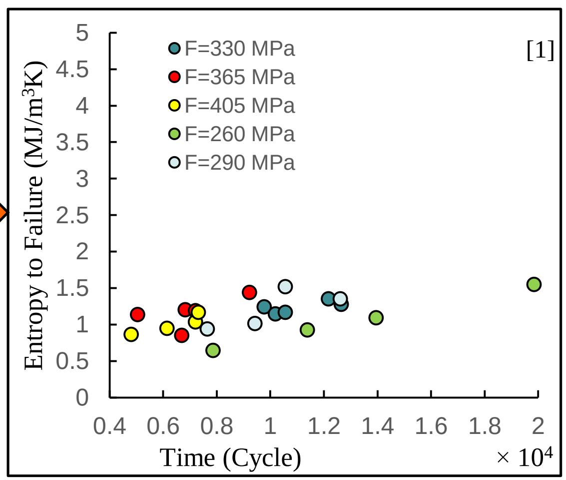
[1] J. Lemaitre, "*A Course on Damage Mechanics*", Springer, France, 1996.
[2] C. Woo & D. Li, "*A Universal Physically Consistent Definition of Material Damage",* Int. J. Solids Structure, V30, 1993

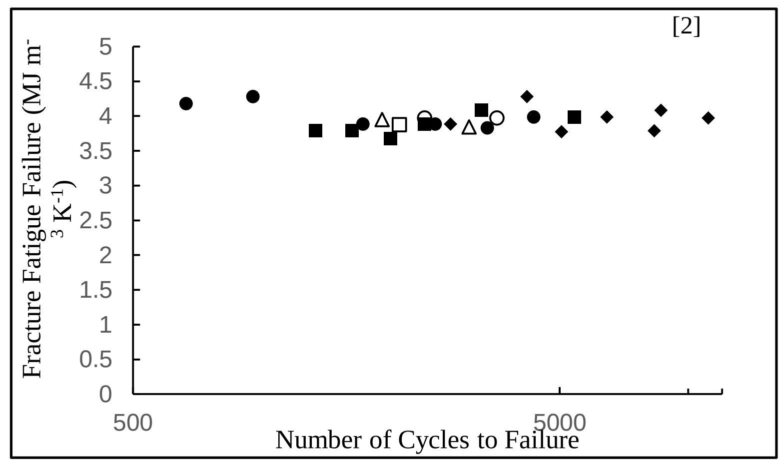
Motivation (Cont.)

Total Strain Energy Expended in 40 P-3 Aircraft with vastly Different Loading Histories when the Miner's Cumulative Damage Reaches 0.5



Entropy to crack initiation





Entropy to Fracture

[1] Anahita Imanian and Mohammad Modarres, A Thermodynamic Entropy Approach to Reliability Assessment with Application to Corrosion Fatigue, Entropy 17.10 (2015): 6995-7020
[2] M. Naderi et al., On the Thermodynamic Entropy of Fatigue Fracture, Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences, 466.2114 (2009): 1-16

Thermodynamics Approach to Damage

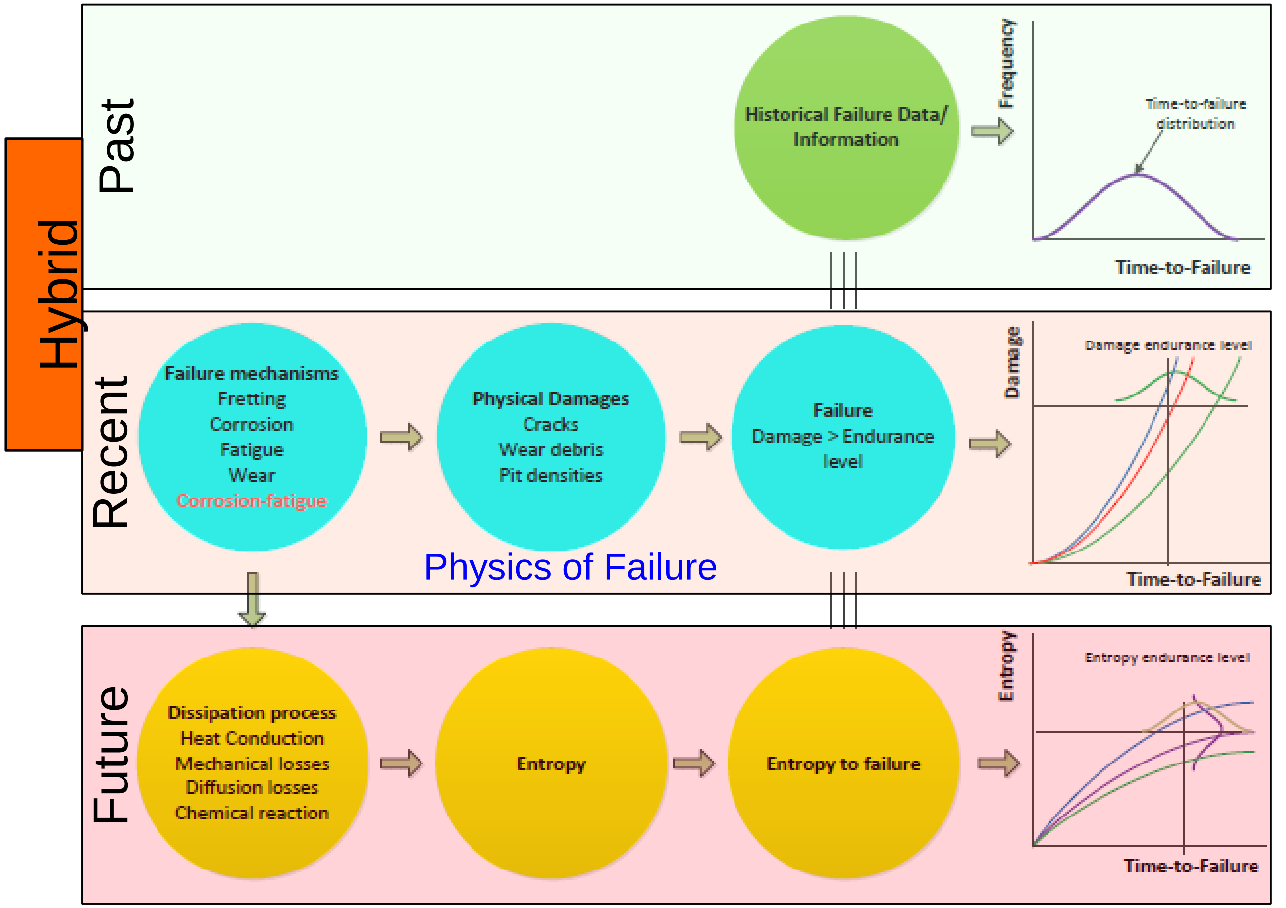
Second Law of Thermodynamics: In an isolated system, entropy will always increase until it reaches a maximum value.

Second Law of Thermodynamics (Statistical Mechanics Version): In an isolated system, the system will always progress to a macrostate that corresponds to the maximum number of microstates.

All damages resulting from failure mechanisms share a common feature: Dissipation of Energy.

Dissipation: a fundamental determinant of irreversibility can be described well within the context of non-equilibrium thermodynamics.

Thermodynamics as the Science of Reliability



Why Entropy?

- ✓ Entropy is independent of the path to failure ending at similar total entropy at failure
- ✓ Entropy accounts for complex synergistic effects of interacting failure mechanisms
- ✓ Entropy is scale independent

An Entropic Theory of Damage

Degradation mechanisms → Damage → Dissipation energies → Entropy generation

Damage ≡ Entropy

An entropic theory follows[1]:

Failure occurs when the accumulated total entropy generated exceeds the entropic-endurance of the unit

- Entropic-endurance describes the capacity of the unit to withstand entropy
- Entropic-endurance of identical units is equal
- Entropic-endurance of different units is different
- Entropic-endurance to failure can be measured (experimentally) and involves stochastic variability

- In this context we define Damage as: $D = \frac{\gamma_d - \gamma_{d_0}}{\gamma_{d_E} - \gamma_{d_0}}$

Entropy generation, γ_d, monotonically increases starting at time zero from a theoretical value of zero or practically some initial entropy, γ_0, to an entropic-endurance value, γ_d

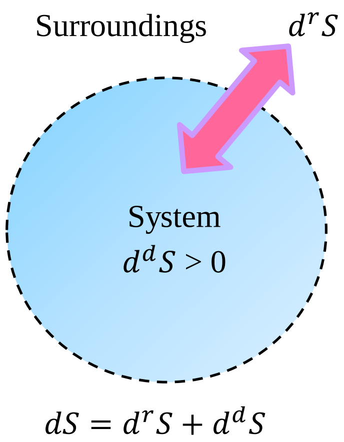
[1] Anahita Imanian and Mohammad Modarres, A Thermodynamic Entropy Approach to Reliability Assessment with Application to Corrosion Fatigue, Entropy 17.10 (2015): 6995-7020

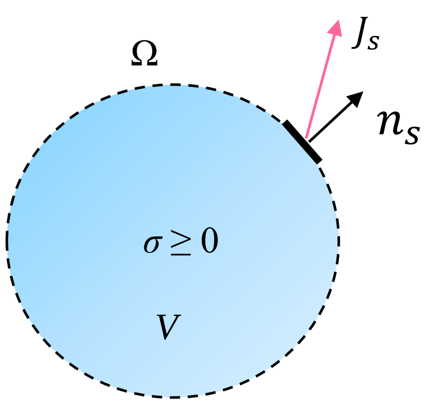
Total Entropy

- 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: $\frac{d^r S}{dt} = -\int^{\Omega} \boldsymbol{J}_s . \boldsymbol{n}_s dA$

  $d^d S$ = irreversible part of the entropy produced inside of the system: $\frac{d^d S}{dt} = \int^{V} \sigma dV$.





- Divergence theorem leads to: $\frac{ds}{dt} + \nabla . \boldsymbol{J}_s = \sigma$, where, s is the specific entropy per unit mass.
- Damage, D, according to our theory is expressed by the entropy generated: $D|t \sim \int_0^t [\sigma | X_i(u), \boldsymbol{J}_i(u)] du$

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

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

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

For near equilibrium condition interactions between multiple dissipation processes is captured by the Onsagar reciprocal relations define forces and fluxes. $J_i = \sum_j L_{ij} X_j$ *For example for Fatigue (f) and Corrosion (c)*

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

$[L_{ij}]$= Onsager matrix of phenomenological coefficients

- Entropy generation of important dissipation phenomena leading to damage:

Thermal energy | Diffusion energy | Plastic deformation energy

$$\sigma = \frac{1}{T^2} \boldsymbol{J}_q . \nabla T + \Sigma_{k=1}^{n} \boldsymbol{J}_k \left(\nabla \frac{\mu_k}{T} \right) + \frac{1}{T} \boldsymbol{\tau} : \dot{\boldsymbol{\epsilon}}_p + \frac{1}{T} \Sigma_{j=1}^{r} v_j\ A_j + \frac{1}{T} \Sigma_{m=1}^{h} c_m \boldsymbol{J}_m (-\nabla \psi)$$

Chemical reaction energy | External fields energy

$\boldsymbol{J}_n$ $(n = q, k, and\ m)$ = thermodynamic fluxes due to heat conduction, diffusion and external fields, T=temperature, μ_k = chemical potential, v_i =chemical reaction rate, $\boldsymbol{\tau}$ =stress tensor, $\dot{\boldsymbol{\epsilon}}_p$ =the plastic strain rate, A_j =the chemical affinity or chemical reaction potential difference, ψ =potential of the external field, and c_m =coupling constant *, **

* D. Kondepudi and I. Prigogine, *"Modern Thermodynamics: From Heat Engines to Dissipative Structures,"* Wiley, England, 1998.

** J. Lemaitre and J. L. Chaboche, "*Mechanics of Solid Materials,*" 3rd edition; Cambridge University Press: Cambridge, UK, 2000.

Examples of Force and Flux of Dissipative Processes

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

Primary mechanism	Thermodynamic force, X	Thermodynamic flow, J	Examples of materials damage process
Heat conduction	Temperature gradient, $\nabla(1/T)$	Heat flux, $\boldsymbol{q}$	Fatigue, creep, wear
Plastic deformation of solids	Stress, $\boldsymbol{\sigma}/T$	Plastic strain, $\dot{\boldsymbol{\varepsilon}}_p$	Fatigue, creep, wear
Chemical reaction	Reaction affinity, A_k/T	Reaction rate, v_k	Corrosion, wear
Mass diffusion	Chemical potential, $-\nabla(\mu_k/T)$	Diffusion flux, $\boldsymbol{J}_k$	Wear, creep
Electrochemical reaction	Electrochemical potential, $\tilde{A}/T$	Current density, i_{corr}/z	Corrosion
Irradiation	Particle flux density, A_r/T	Velocity of target atoms after collision, $\dot{v}_r$	Irradiation damage
Annihilation of lattice sites	Creep driving force $(\tilde{\boldsymbol{\sigma}} - \omega \boldsymbol{I})/T$	Creep deformation rate, $\boldsymbol{R}$	Creep

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

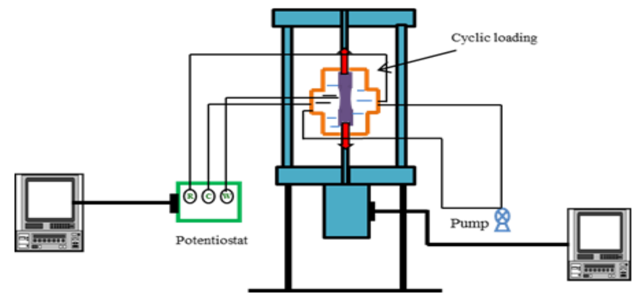
Entropic-Based Damage from Corrosion-Fatigue (CF)

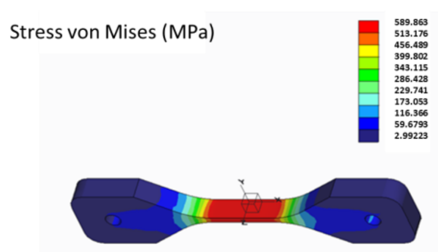
- Oxidation and reduction reactions of metallic electrode, M, under CF:

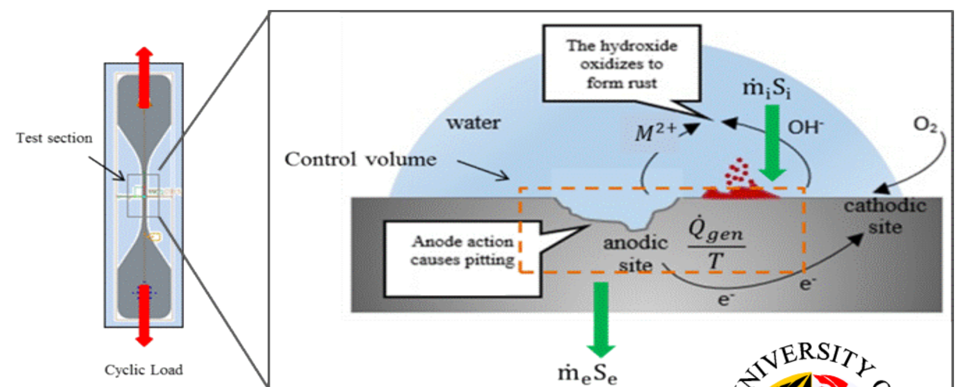
$$M \leftrightarrow M^{z_M^+} + z_M e^-$$
$$O + z_O e^- \leftrightarrow R$$

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

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







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

$$\sigma = \frac{1}{T}\left(\boldsymbol{J}_{M,a} z_M F E_{M_{act,a}} + \boldsymbol{J}_{M,c} z_M F E_{M_{act,c}} + \boldsymbol{J}_{O,a} z_O F E_{O_{act,a}} + \boldsymbol{J}_{O,c} z_O F E_{O_{act,c}}\right)$$

$$+ \frac{1}{T}\left(\boldsymbol{J}_{M,c} z_M F E_{M_{conc,c}} + z_O F \boldsymbol{J}_{O,c} E_{O_{conc,c}}\right)$$

Diffusion dissipations

$$+ \frac{1}{T}\left(\boldsymbol{J}_{M,a}\alpha_M A_M + J_{M,c}(1-\alpha_M)A_M + \boldsymbol{J}_{O,a}\alpha_O A_O + \boldsymbol{J}_{M,a}(1-\alpha_O)A_O\right)$$

Chemical reaction dissipations

$$+ \frac{1}{T}\dot{\boldsymbol{\epsilon}}_p : \boldsymbol{\tau} + \frac{1}{T} Y \dot{\boldsymbol{D}}$$

Mechanical dissipations

$$+\sigma_H$$

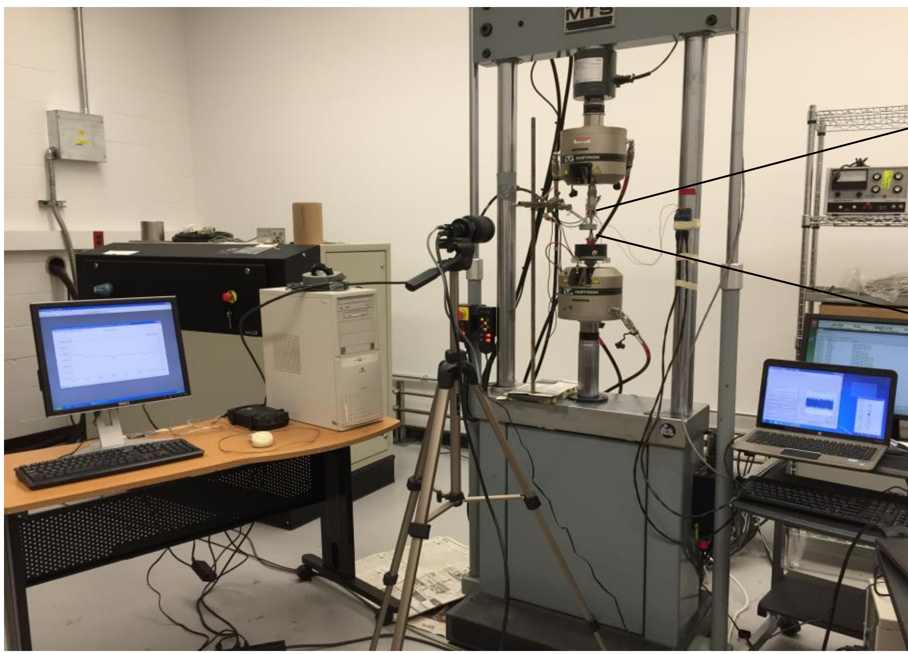
Hydrogen embrittlement dissipation

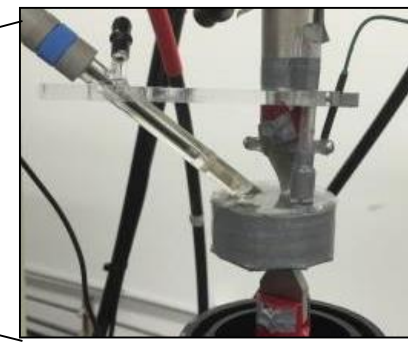
T = temperature, z_M =number of moles of electrons exchanged in the oxidation process, F =Farady number, $J_{M,a}$ and $J_{M,c}$ = irreversible anodic and cathodic activation currents for oxidation reaction, $J_{O,a}$ and $J_{O,c}$ =anodic and cathodic activation currents for reduction reaction, $E_{M_{act,a}}$ 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 reduction reaction, $E_{M_{conc,c}}$ and $E_{O_{conc,c}}$ =concentration over-potentials for the cathodic oxidation and cathodic reduction reactions, α_M and α_O =charge transport coefficient for the oxidation and reduction reactions, A_M and A_O = chemical affinity for the oxidation and reductions, $\dot{\epsilon}_p$ =plastic deformation rate, τ =plastic stress, $\dot{D}$ =dimensionless damage flux, Y the elastic energy, and σ_H =entropy generation due to hydrogen embrittlement.

Corrosion Fatigue (CF) 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

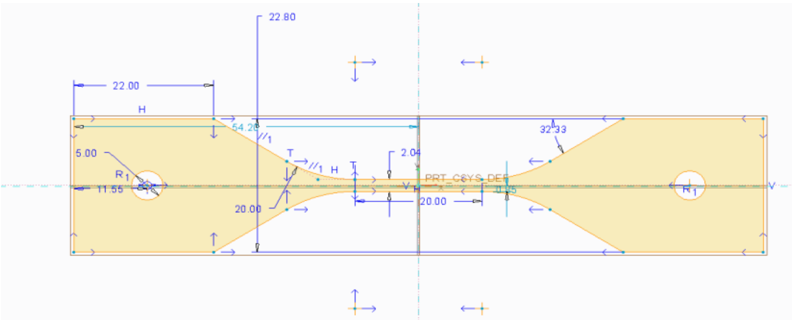
CF tests done while measuring the open circuit potential (OCP) vs. reference electrode during load-unload





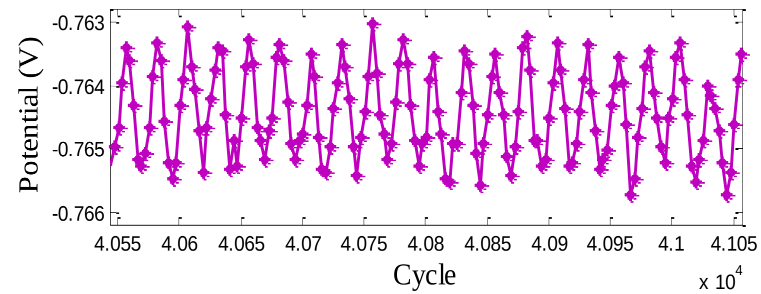
Electrochemical corrosion cell made of plexiglass

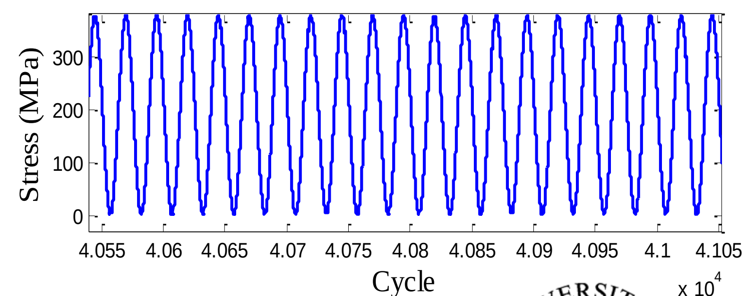
CF Test Procedures



Forces and fluxes were measured under CF

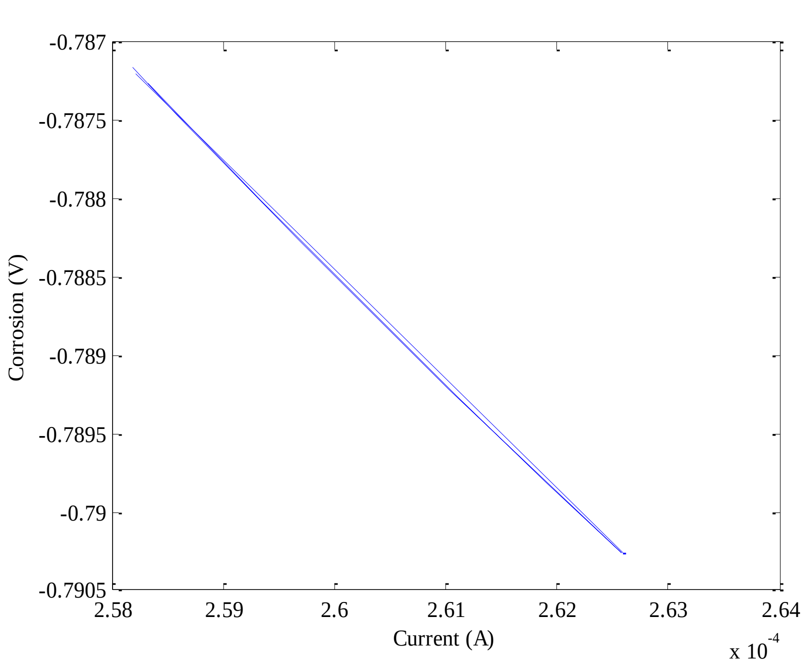
- Performed CF tests for 16 samples at 87%, 80%, 70% and 57% of yield stress (460 MPa), load ratio = 0.01, loading frequency=0.04Hz
- Tests stopped after failure of specimens

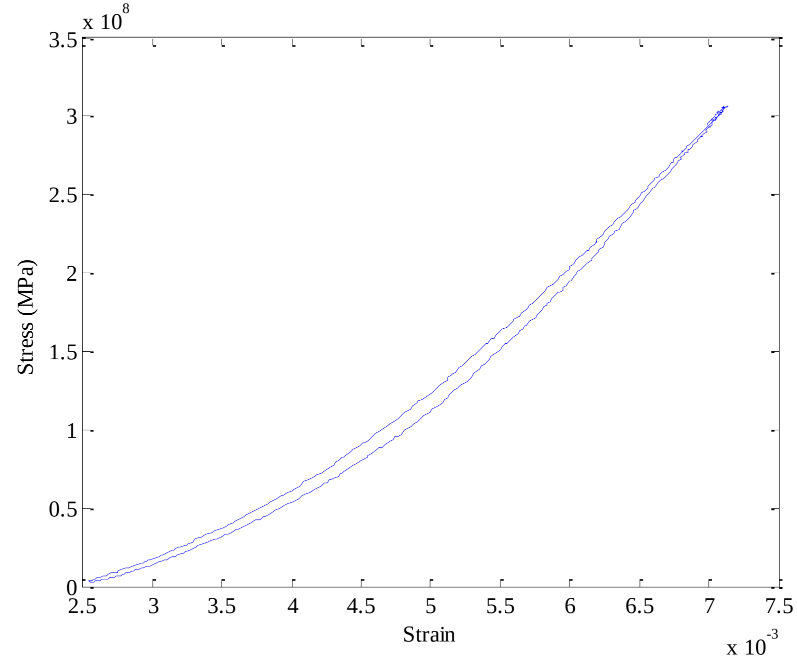




Entropy Generation in CF

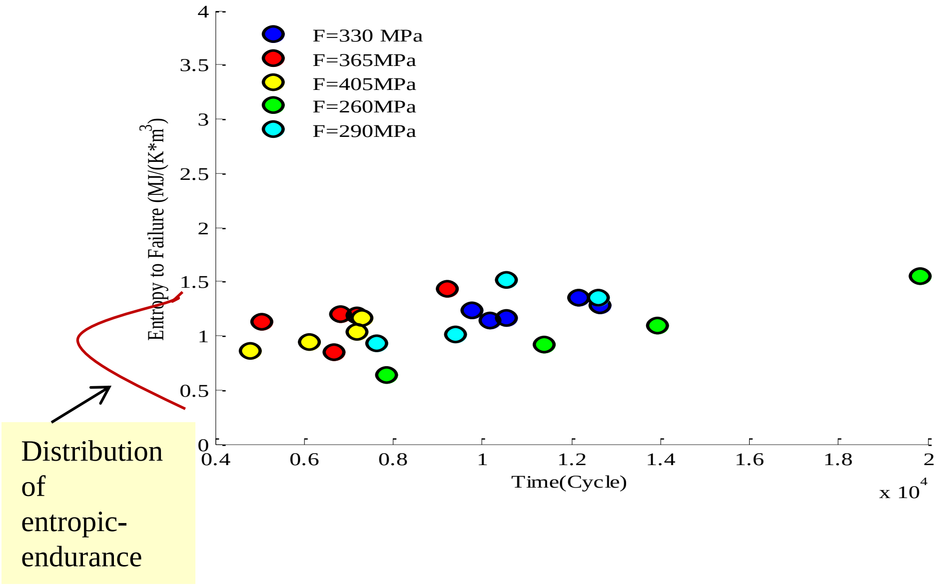
- Total entropy is measured from the hysteresis loops resulted from fatigue (stress-strain) and corrosion (potential-electrical) in each loading cycle

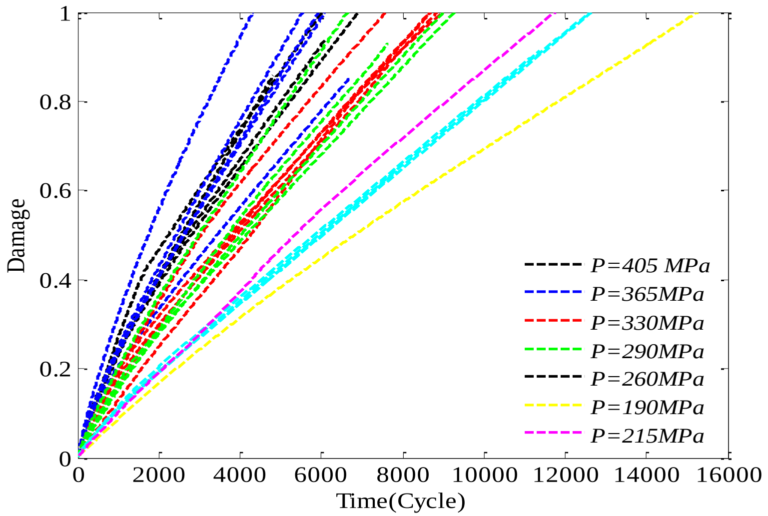




Entropic Endurance and Entropy-to-Failure

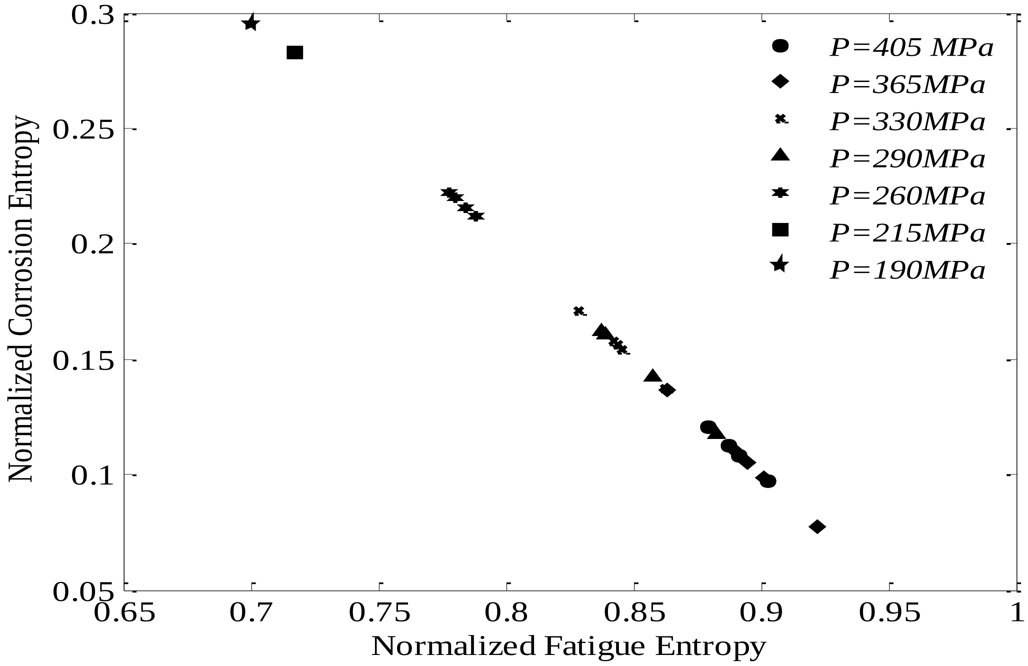
- Similarity of the total entropy-to-failure for all tests supports the entropic theory of damage offered proposed
- More tests needed to reduce the epistemic uncertainties and further confirm the theory





Ratio of Corrosion and Fatigue Entropies to the Total Entropy

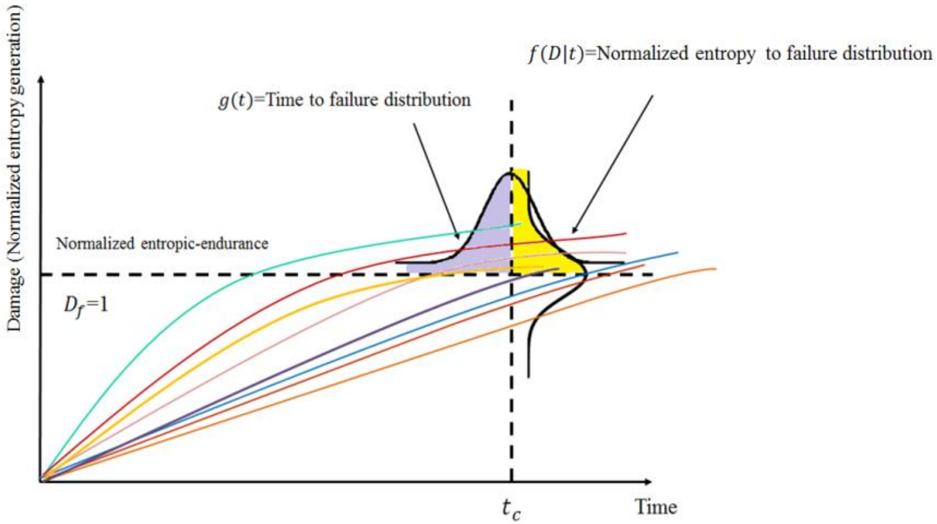
- Reducing fatigue stress allows more time for corrosion



Thermodynamics of Damage: A Reliability Perspective

- Materials, environmental, operational and other types of variabilities in degradation forces impose uncertainties on the total entropic damage

- Assuming a constant *entropic-endurance*, D_f



- The reliability function can be expressed as [1]

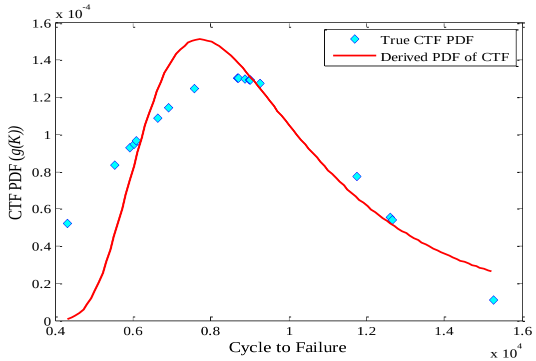
$$P_r(T \leq t_c) = \int_0^{t_c} g(t)dt = 1 - \int_0^{D_f=1} f(D)dD$$

$$R(t_c) = 1 - P_r(T \leq t_c) = \int_0^{D_f=1} f(D)dD$$

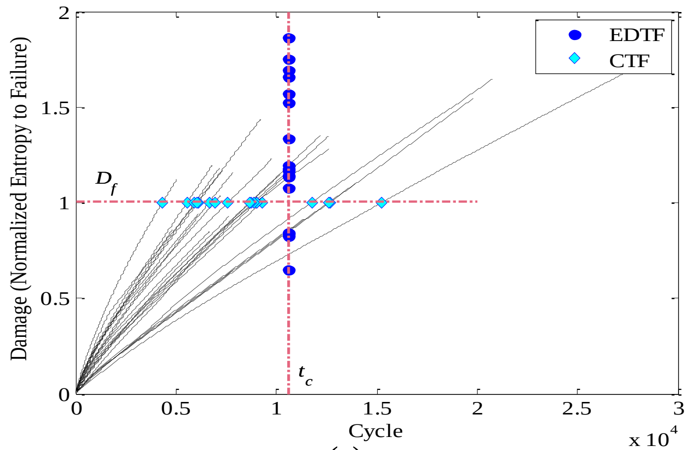
T_c =*Current operating time;* $g(t)$=*distribution of time-to-failure,* $f(D|t)$= *distribution of damage at t*

[1] Thermodynamics as a Fundamental Science of Reliability, A. Imanian, M. Modarres, Int. J. of Risk and Reliability, Vol.230(6), pp.598-608. DOI: 10.1177/1748006X16679578.(2016).

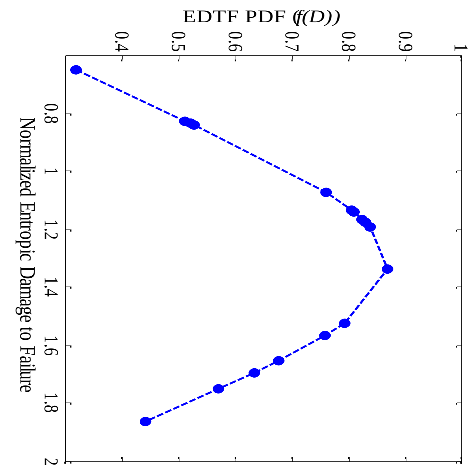
Entropic-Based CF Reliability



(c)



(a)



(b)

Conclusions

- A thermodynamic theory of damage proposed and tested
- An entropy-based damage model derived from the second law of thermodynamics and used it to develop models for reliability analysis
- The proposed theory offered a more fundamental model of damage and allowed for incorporation of all interacting dissipative processes
- Entropy generation function derived for corrosion-fatigue mechanism in terms of leading dissipative processes
- A simplified version of entropic corrosion-fatigue damage model experimentally studied which supported the proposed theory and the thermodynamic-based interpretation of reliability

Thank you

Approaches to derive and quantify entropy

Entropy

Statistical mechanics

$$S = K_B \ln W$$

$$\Delta S_i(W) = k_B \log \frac{\pi_{F,i}(+W)}{\pi_{R,i}(-W)}$$

Classical Thermodynamics and Continuum mechanics

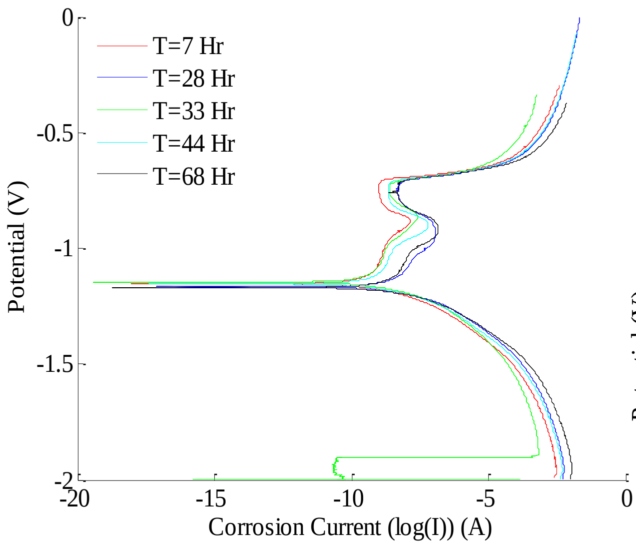
$$\sigma = \frac{1}{T^2} \boldsymbol{J}_q . \nabla T - \Sigma_{k=1}^{n} \boldsymbol{J}_k \left(\nabla \frac{\mu_k}{T} \right) + \frac{1}{T} \boldsymbol{\tau} : \dot{\boldsymbol{\epsilon}}_p + \frac{1}{T} \Sigma_{j=1}^{r} v_j \, A_j + \frac{1}{T} \Sigma_{m=1}^{h} c_m \boldsymbol{J}_m (-\nabla \psi)$$

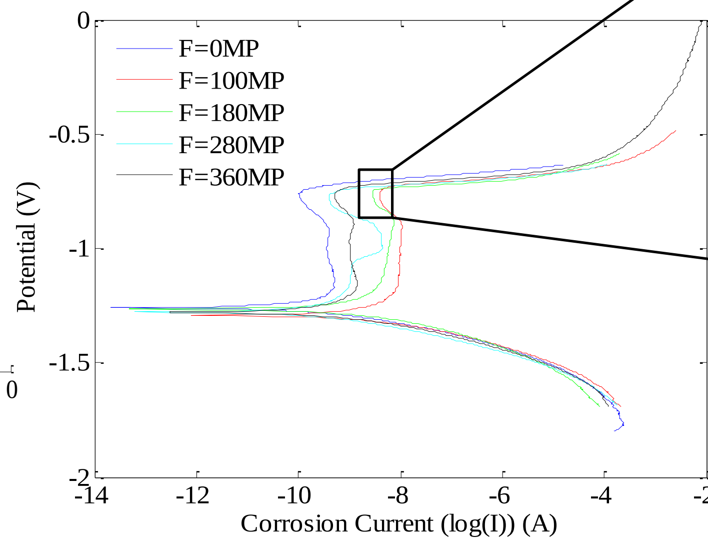
Information Theory

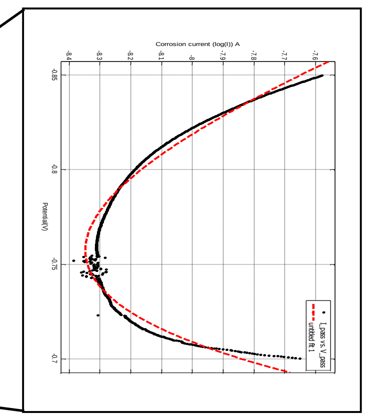
$$S = \sum p_i \log p_i$$

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., $J_i(X_j)$