

# Entropic Damage: A New Physics-of-Failure and Prognosis Perspective

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# Acknowledgments

## The Team:

1. Mr. Huisung Yun (Current PhD candidate)
2. Dr. Anahita Imanian (Former PhD Student)
3. Dr. Victor Ontiveros (Former PhD Student)
4. Ms. Christine Sauerbrunn (Former MS Student)
5. Dr. Mehdi Amiri (Former Postdoc)
6. Dr. Ali Kahirdeh (Current Postdoc)
7. Prof. C. Wang (Corrosion/electrolysis consultant)
8. Prof. Enrique Droguett (Adjunct Associate Professor)
9. Prof. Mohammad Modarres (PI)

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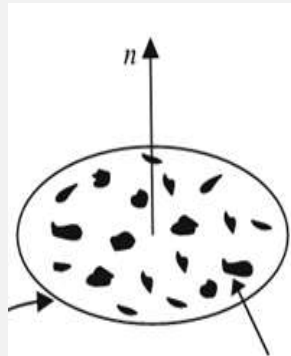


# Objectives

- 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<sup>nd</sup> 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

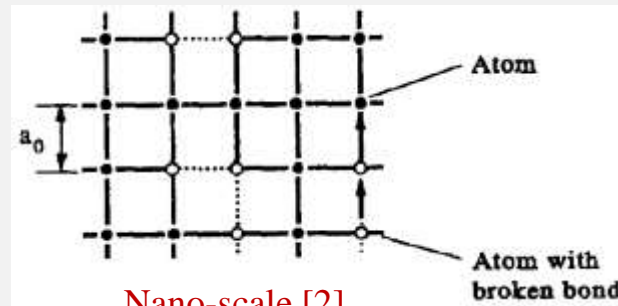
# Motivation

- 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



Continuum damage mechanics [1]

Micro-scale



Nano-scale [2]



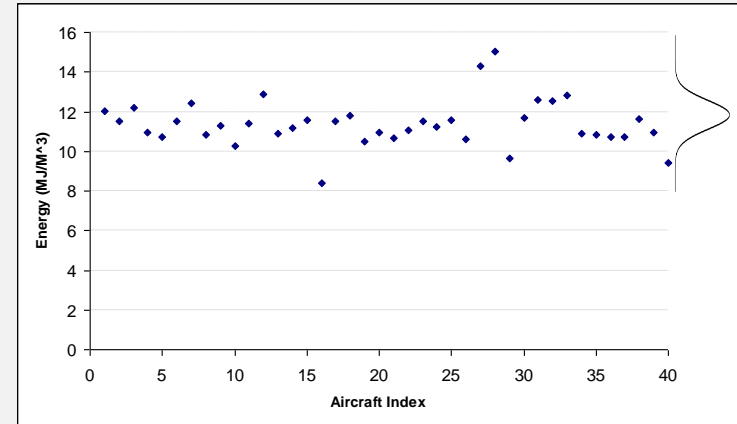
Meso-scale

[1] J. Lemaitre, "A Course on Damage Mechanics", Springer, France, 1996.

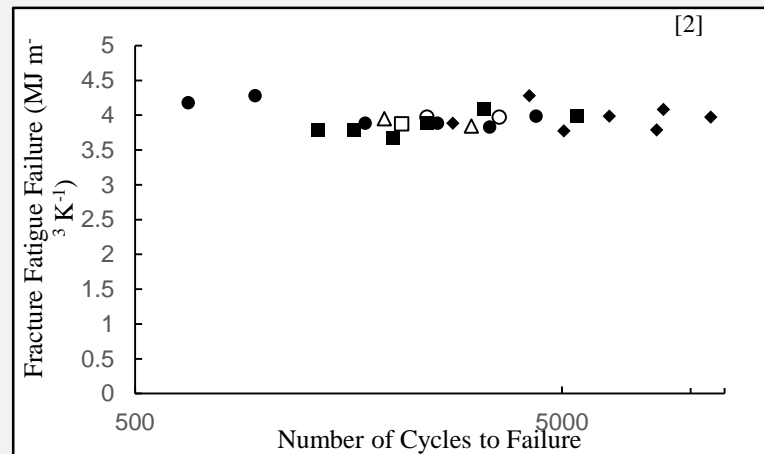
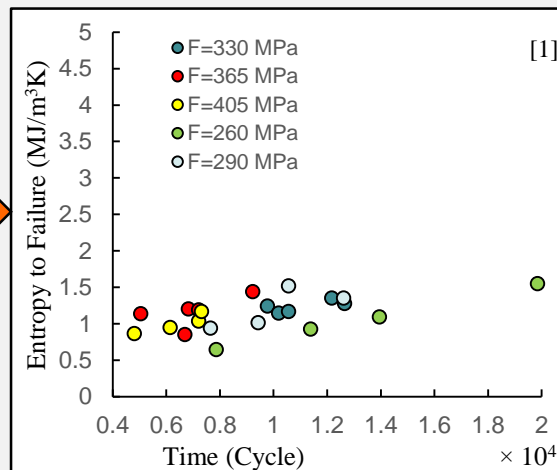
[2] C. Woo & D. Li, "A Universal Physically Consistent Definition of Material Damage", Int. J. Solids Structure, V30, 1993

# 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

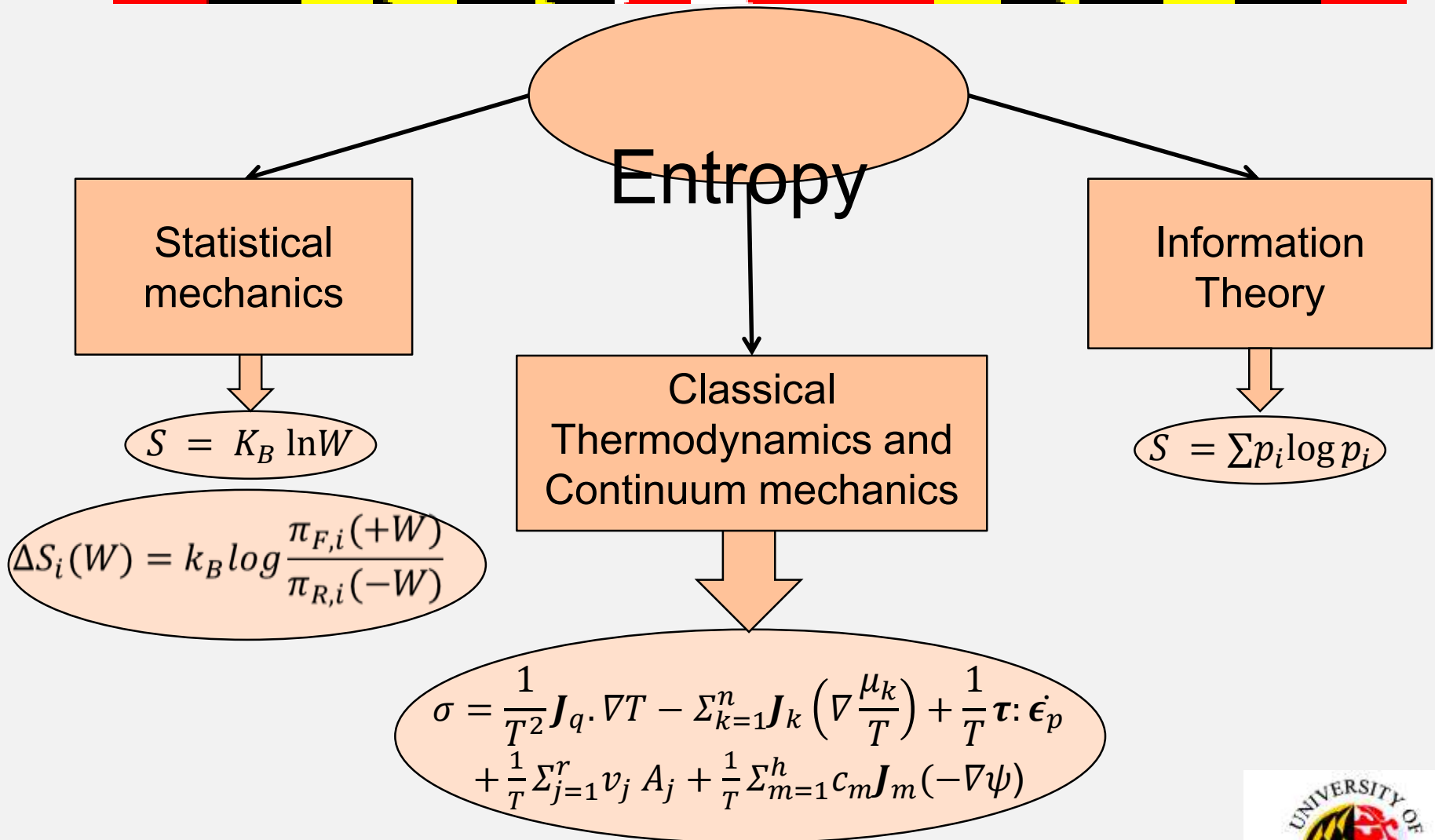
**Second Law of Thermodynamics:** In an isolated system, entropy will always increase until it reaches a maximum value.

**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.

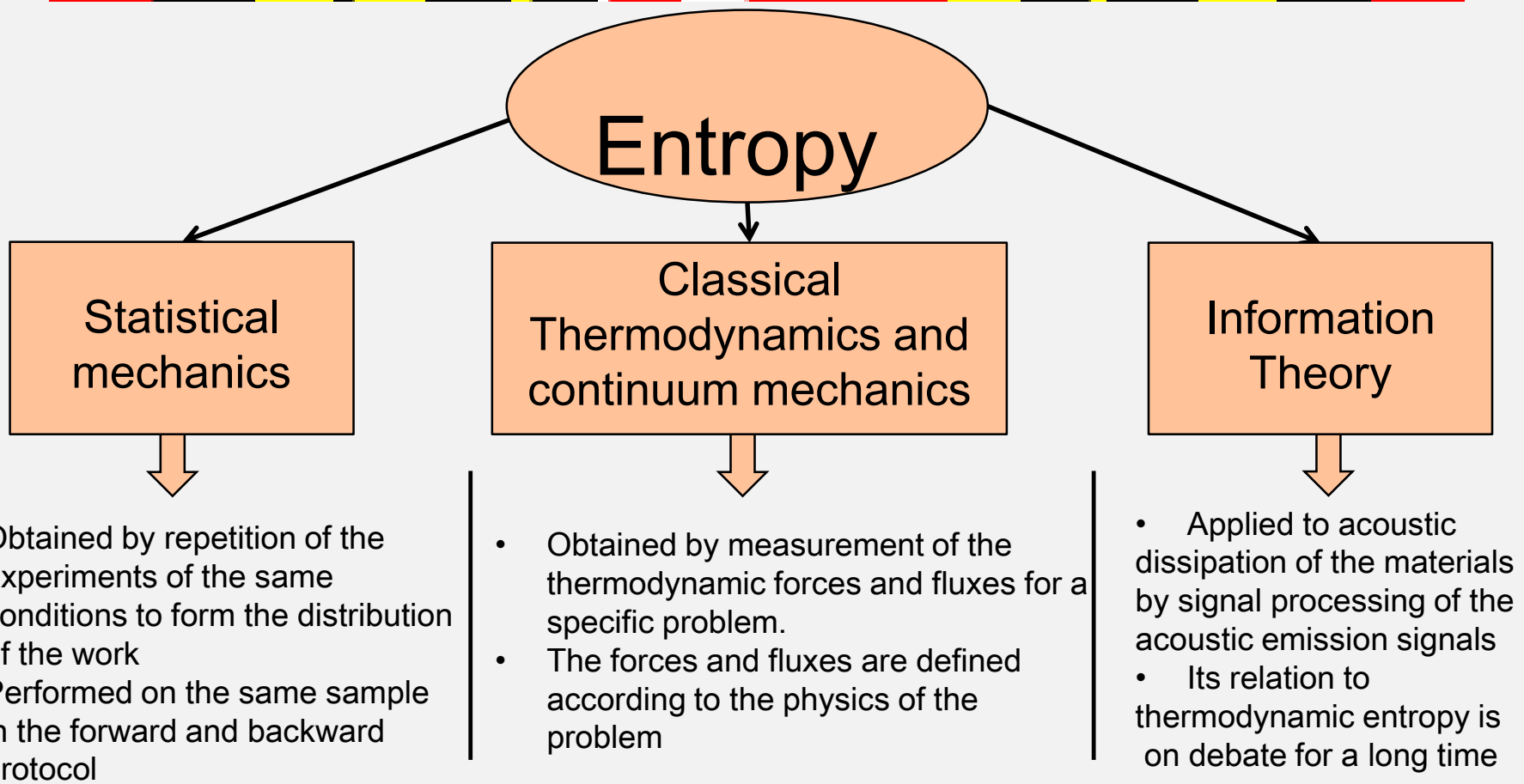
*All damages resulting from failure mechanisms share a common feature: Dissipation of Energy.*

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

# Approaches to derive and quantify entropy



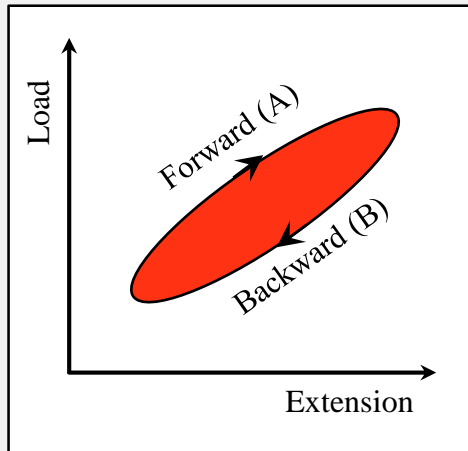
# Approaches to derive and quantify entropy





# Thermodynamic entropy

$$\sigma = \underbrace{\frac{1}{T^2} J_q \cdot \nabla T}_{\text{Heat Conduction}} - \underbrace{\sum_{k=1}^n \left( \nabla \frac{\mu_k}{T} \right)}_{\text{Diffusion}} + \underbrace{\frac{1}{T} \tau : \dot{\epsilon}_p}_{\text{Mechanical}} + \underbrace{\frac{1}{T} \sum_{j=1}^r v_j A_j}_{\text{Chemical}} + \underbrace{\frac{1}{T} \sum_{m=1}^h c_m J_m (-\nabla \psi)}_{\text{External field energy}} \quad [1]$$

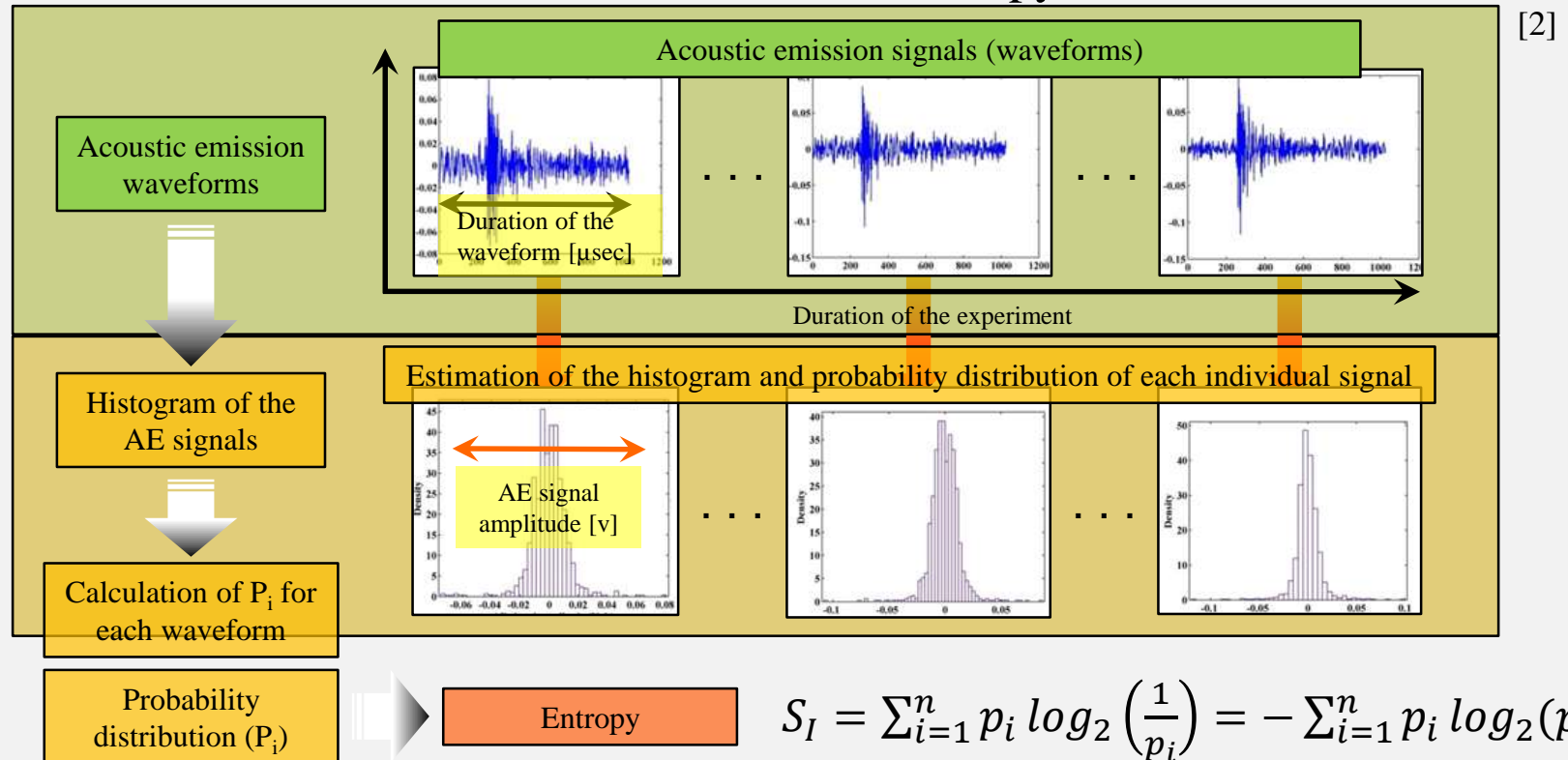


$$\Delta S_{total} = \frac{W^{diss}}{T} = \frac{\text{Hysteresis Area}}{T}$$

Hysteresis Area: From load-extension analysis  
T: From surface temperature measured by infrared camera

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

## ➤ Acoustic emission waveform information entropy



[2] Ali Kahirdeh et al., Acoustic Emission Entropy as a Measure of Damage in Materials, Bayesian Inference and Maximum Entropy Methods in Science and Engineering AIP Conf. Proc. 1757 (2016): 060007-1-7



## Approaches to Estimate from AE Signals

### Discrete approaches

Acoustic emission waveforms



Histogram of the AE signals



Calculation of  $p_i$  each waveform



Probability distribution ( $p_i$ )



Shannon Entropy

$$S_E = - \sum_{i=1}^n p_i \log_2(p_i)$$

### Parametric approach

Acoustic emission waveforms



Assigning a set of trial probability density function to the acoustic waveform



Model selection based on the Maximum Entropy obtained

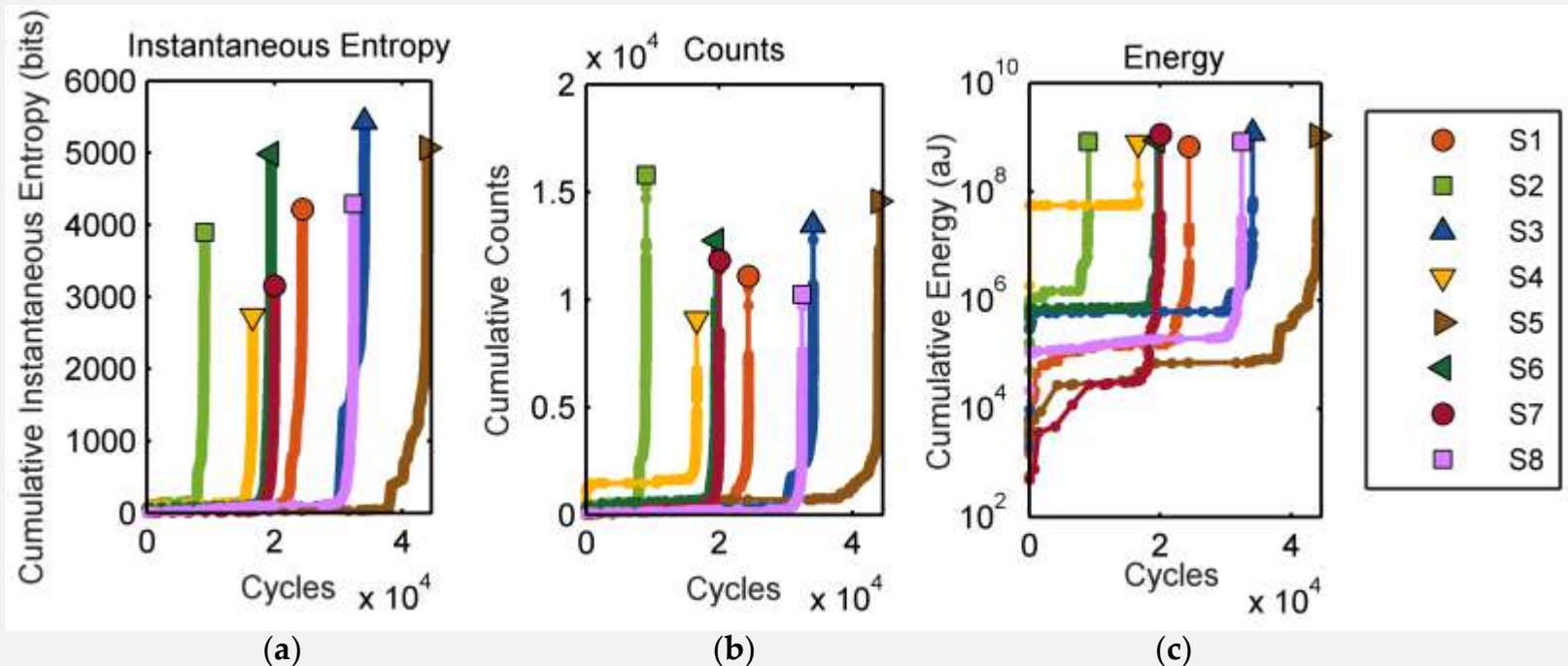


Shannon Entropy

$$S = - \int_{-\infty}^{+\infty} f(x) \log[f(x)] dx$$

► Includes feature, updated, relative, and Bayesian entropy approaches

# Information Entropy

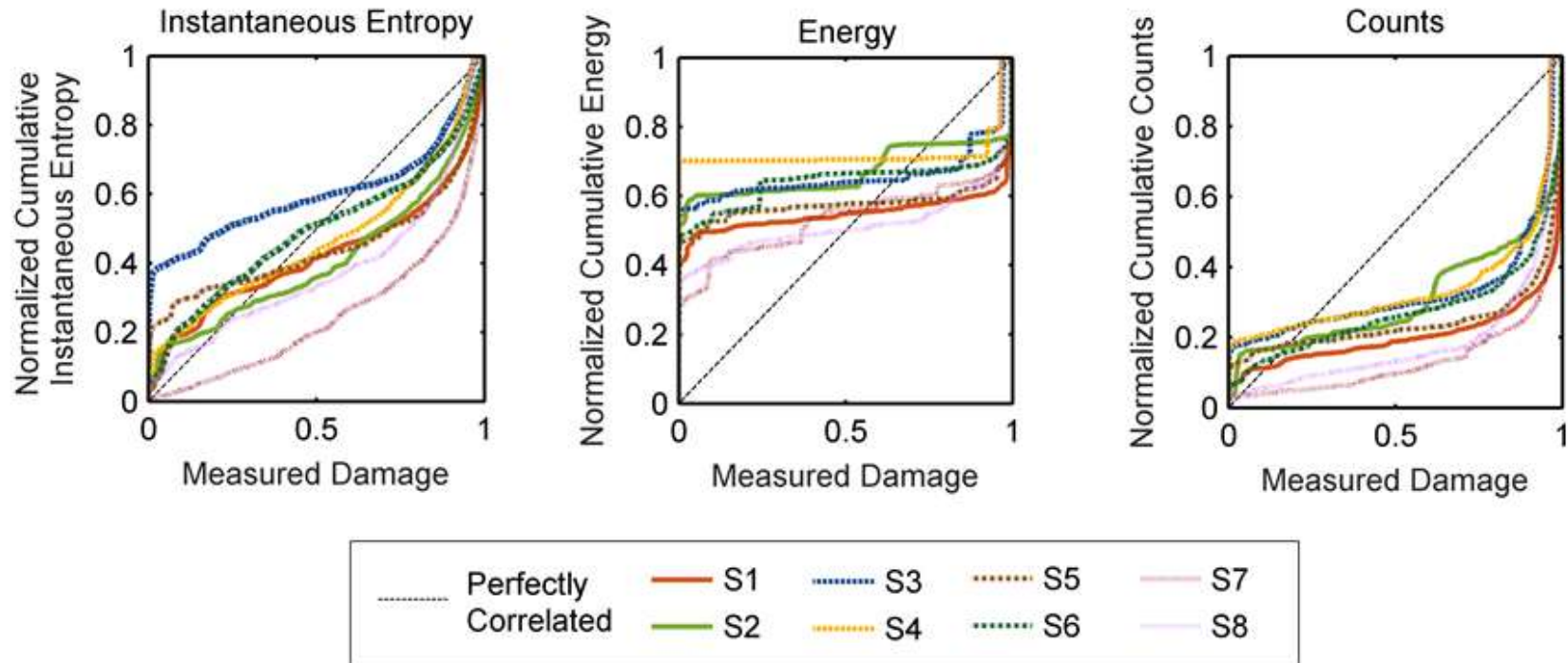


**Figure 5.** Cumulative trend for 3 parameters versus fatigue cycles: (a) Cumulative instantaneous entropy; (b) Cumulative counts; (c) Cumulative energy.

Sauerbrunn, Christine Marie. Evaluation of Information Entropy from Acoustic Emission Waveforms as a Fatigue Damage Metric for Al7075-T6. Diss. 2016.



# Information Entropy of acoustic signals

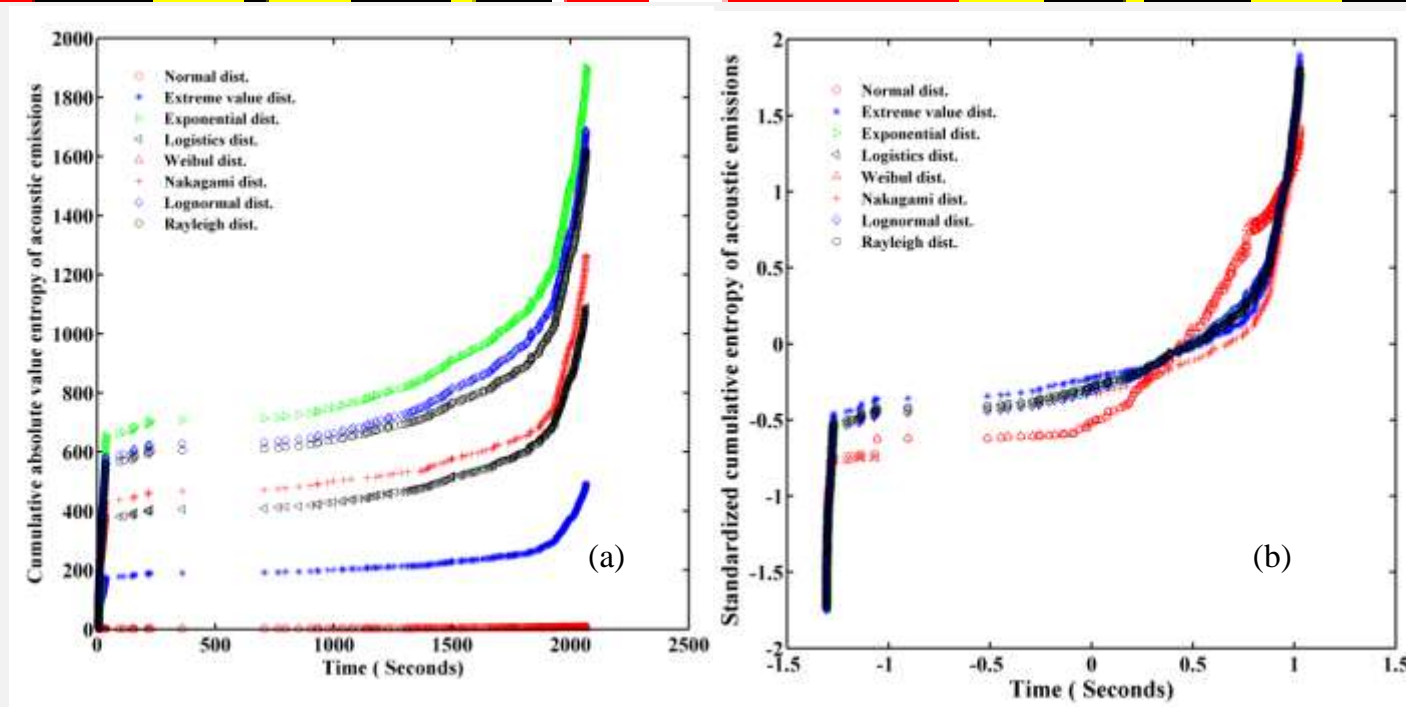


Normalized cumulative trend for 3 parameters with respect to measured damage where a one-to-one relationship is desired: (a) Instantaneous entropy; (b) Counts; (c) Energy.

Sauerbrunn, Christine Marie. *Evaluation of Information Entropy from Acoustic Emission Waveforms as a Fatigue Damage Metric for Al7075-T6*. Diss. 2016.



# Information Entropy (Shannon Entropy) of acoustic signals



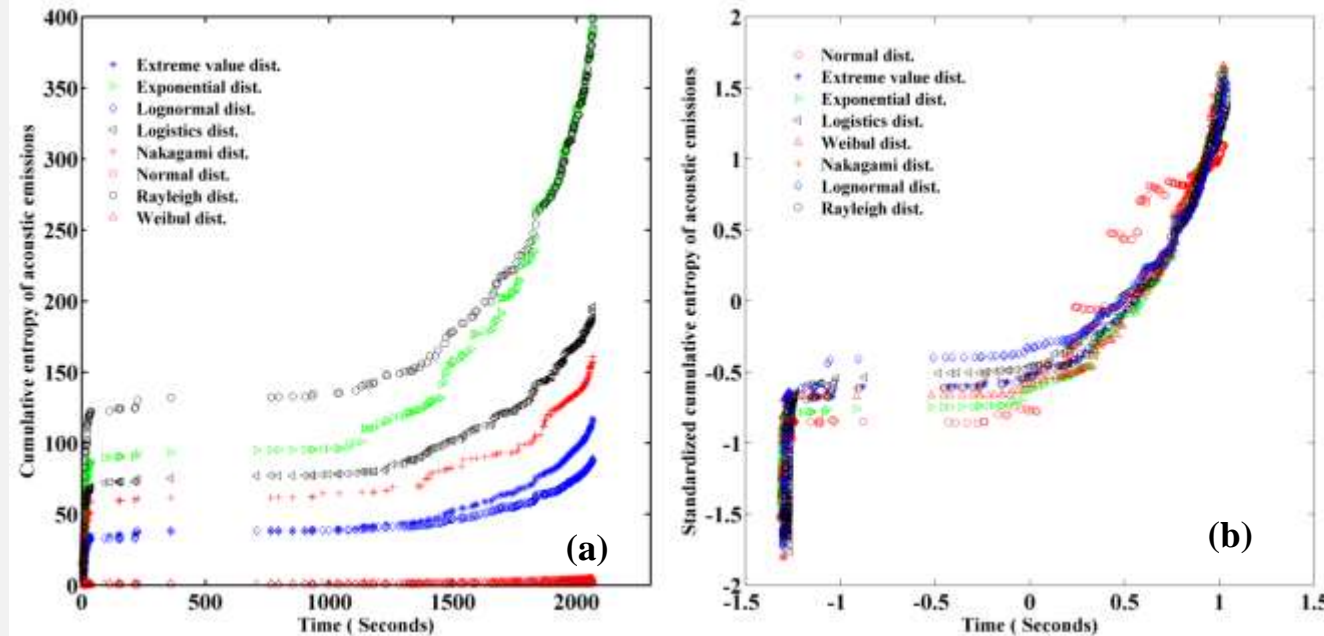
$$I[p(x)] = -k_B \int p(x) \log p(x) dx$$

A) The absolute value of the estimated acoustic emission information entropy. B), The standardized cumulative acoustic emission entropy where the eight graphs related to eight trial probability density function are plotted.

A Parametric Approach to Acoustic Entropy Estimation for Assessment of Fatigue Damage,  
A. Kahirdeh, C. Sauerbrunn, H. Yun, M. Modarres, International Journal of Fatigue (Submitted, 2017).



# Relative entropy of acoustic signals



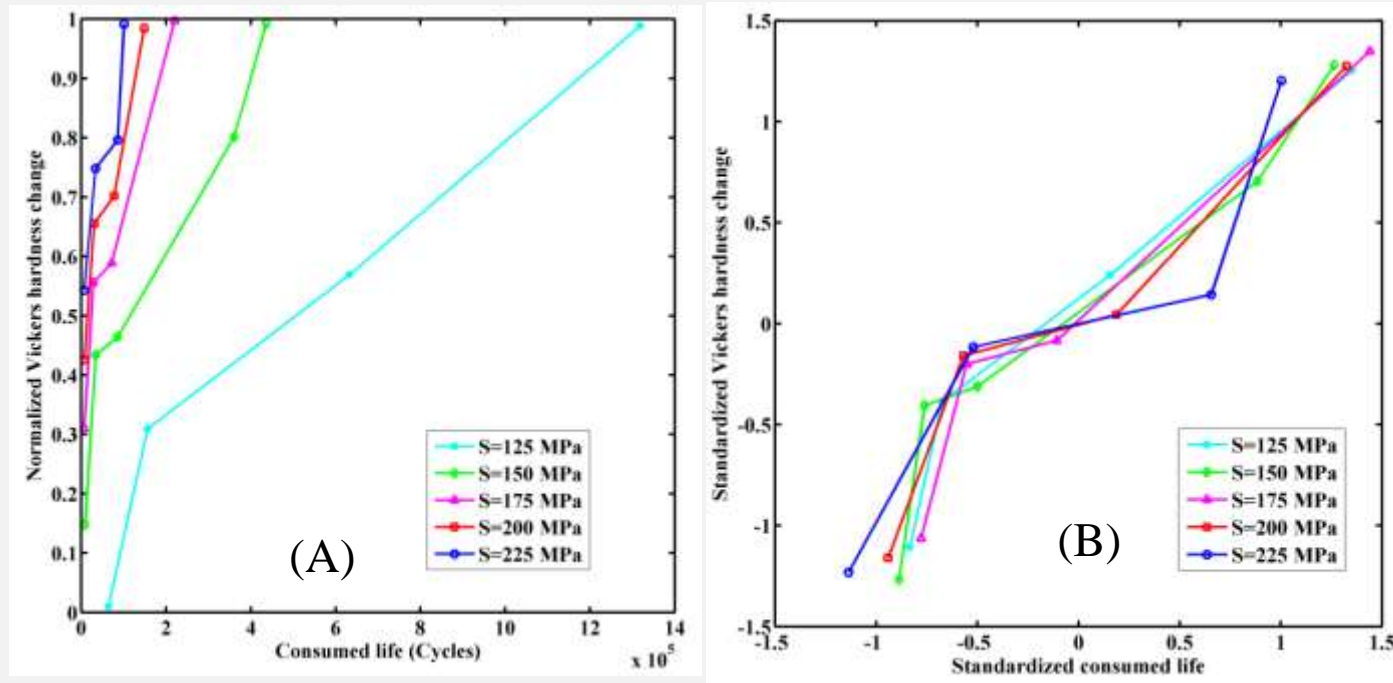
$$S(P|Q) = - \int_{-\infty}^{+\infty} p(x) \log \left( \frac{p(x)}{q(x)} \right) dx \quad \longrightarrow \quad S_i(P|Q) = - \int_{-\infty}^{+\infty} p_i(x) \log \left( \frac{p_i(x)}{p_{i-1}(x)} \right) dx$$

A Parametric Approach to Acoustic Entropy Estimation for Assessment of Fatigue Damage,  
A. Kahirdeh, C. Sauerbrunn, H. Yun, M. Modarres, International Journal of Fatigue (Submitted,  
2017).





# Hardness change prior to crack initiation



A) Hardness change in Al 2024-T42, B) Standardized hardness change in Al 2024-T42. The data of the hardness change are obtained from the study by Pavlou

D.G. Pavlou, A phenomenological fatigue damage accumulation rule based on hardness increasing, for the 2024-T42 aluminum, Engineering Structures, 24 (2002) 1363-1368.

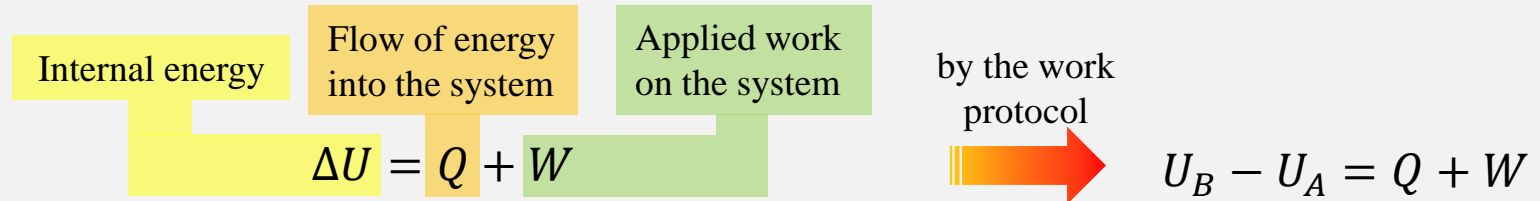




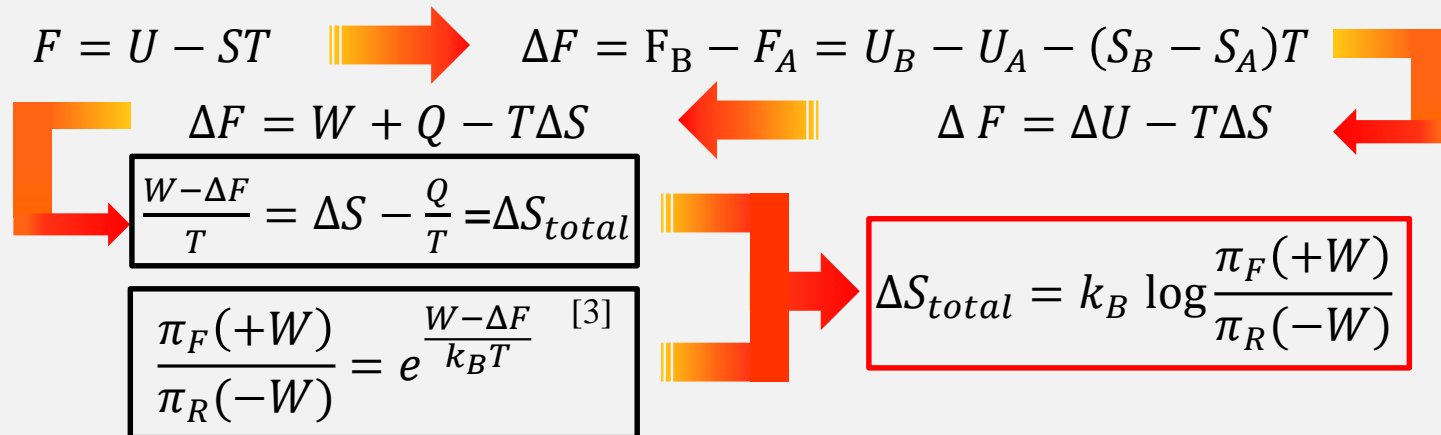
# Statistical Mechanics Entropy

## ➤ Theoretical Basis for Acquiring Entropy

### ➤ First law of thermodynamics



### ➤ From Helmholtz free energy



[3] Crooks, Gavin E. "Entropy production fluctuation theorem and the nonequilibrium work relation for free energy differences." *Physical Review E* 60.3 (1999): 2721.



# Entropy Originated from Statistical Mechanics

- Forward / reverse process representing equations in statistical mechanics

|  |   |
|--|---|
| $\frac{\pi_F(+W)}{\pi_R(-W)} = \exp\left[\frac{W - \Delta F}{k_B T}\right]$ <div style="text-align: center; margin-top: 10px; border: 1px solid black; background-color: #f4a460; padding: 5px; width: fit-content; margin: 0 auto;">Crooks' fluctuation theorem</div> | <div style="text-align: right;">[3]</div> $\frac{W_F^{diss}}{k_B T} = \frac{\langle W_F \rangle - \Delta F}{k_B T} = D(\pi_F   \mu_R) = \int \pi_F \ln\left(\frac{\pi_F}{\pi_R}\right)$ <div style="text-align: center; margin-top: 10px; border: 1px solid black; background-color: #f4a460; padding: 5px; width: fit-content; margin: 0 auto;">Relative entropy</div> |
|--|---|

- In order to define forward / reverse distribution,
- Repeats fatigue test with same (internal & external) condition
  - Collects matching data (e.g. work with same life ratio)

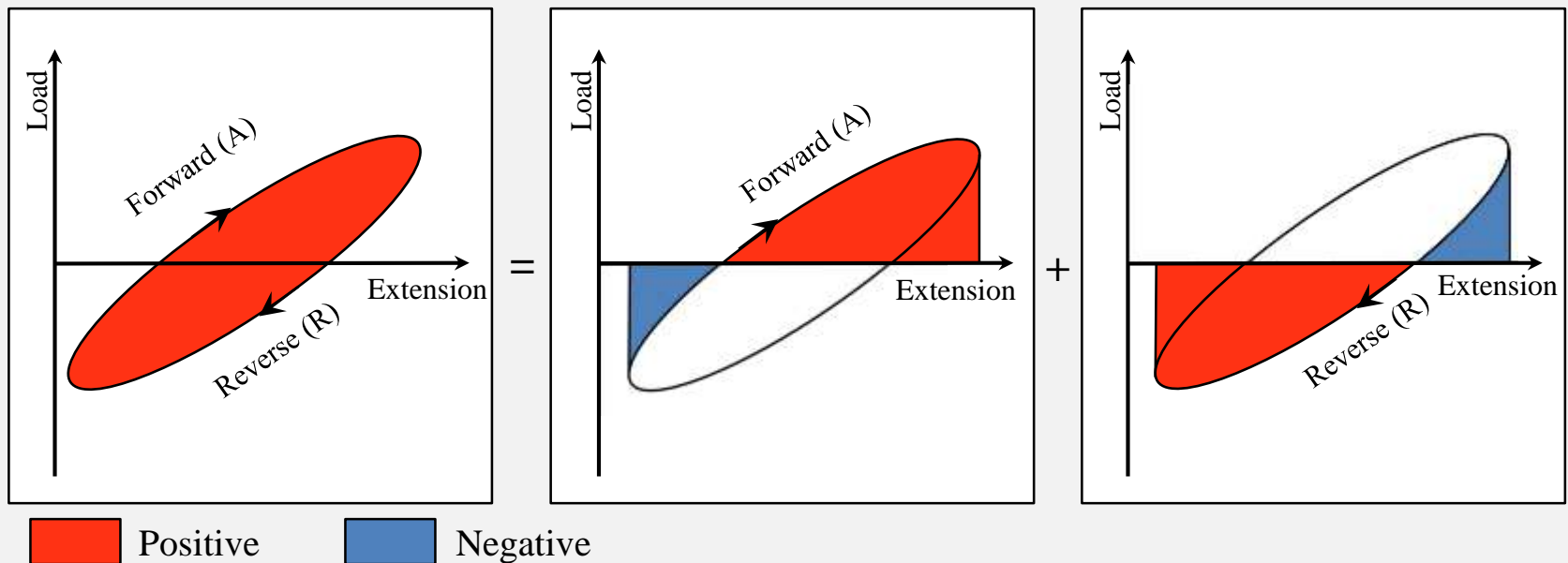
[3] C. Jarzynski, Equalities and Inequalities: Irreversibility and the Second Law of Thermodynamics at the Nanoscale, Annu. Rev. Condens. Matter Phys. 2.1 (2011): 329-351



# Test & Data Arrangement

## Forward / Reverse Work Computation

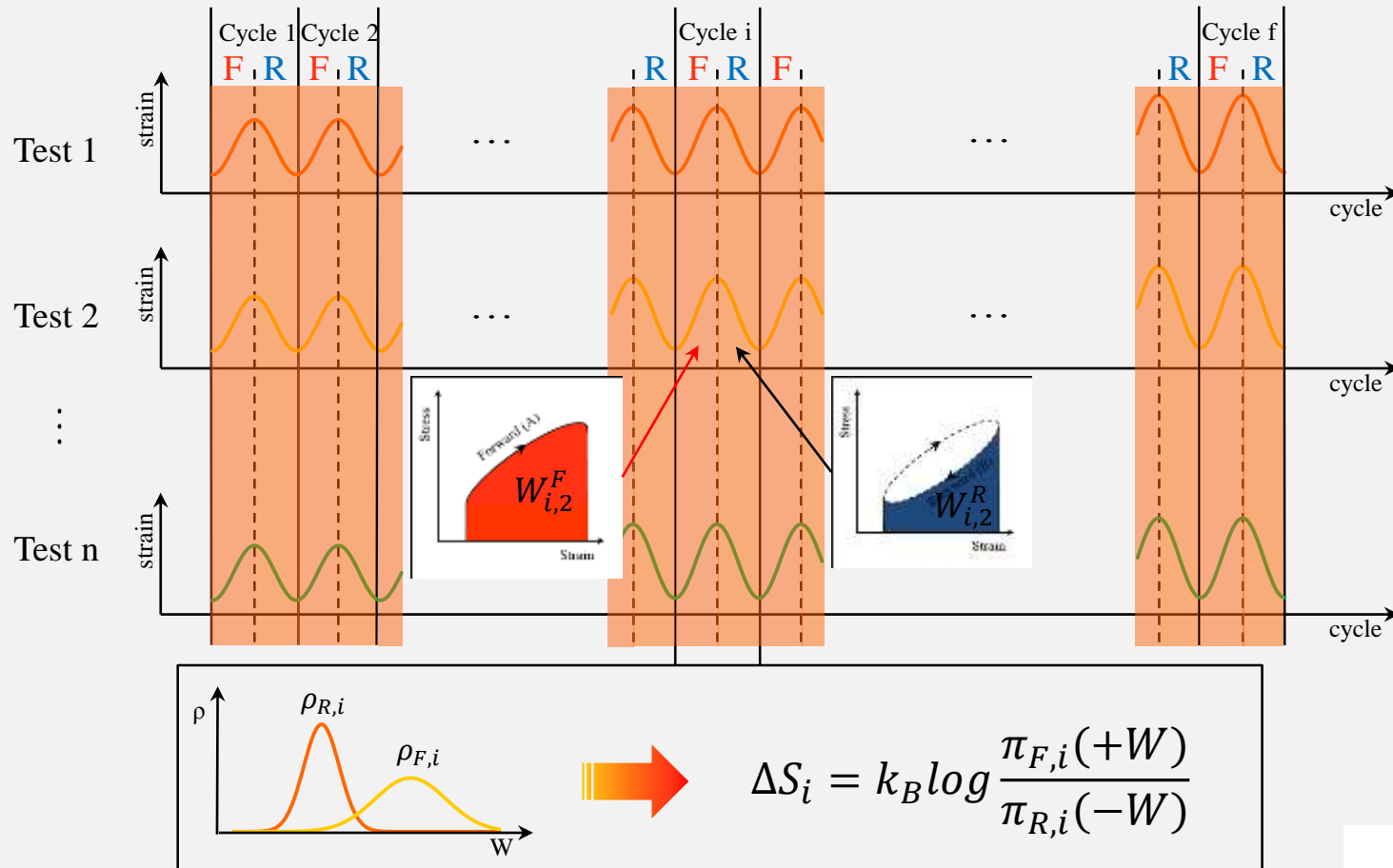
✦ For the fully-reversed fatigue loading condition



✦ Forward and reverse work for each cycle is numerically computed

# Statistical Mechanics Entropy

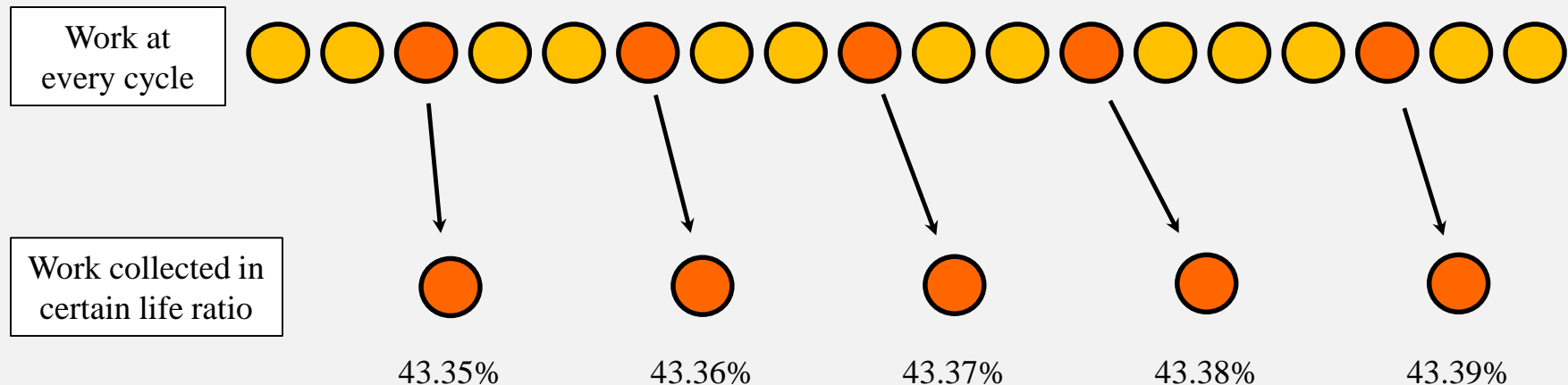
## Schematics of Entropy Computation



# Test & Data Arrangement

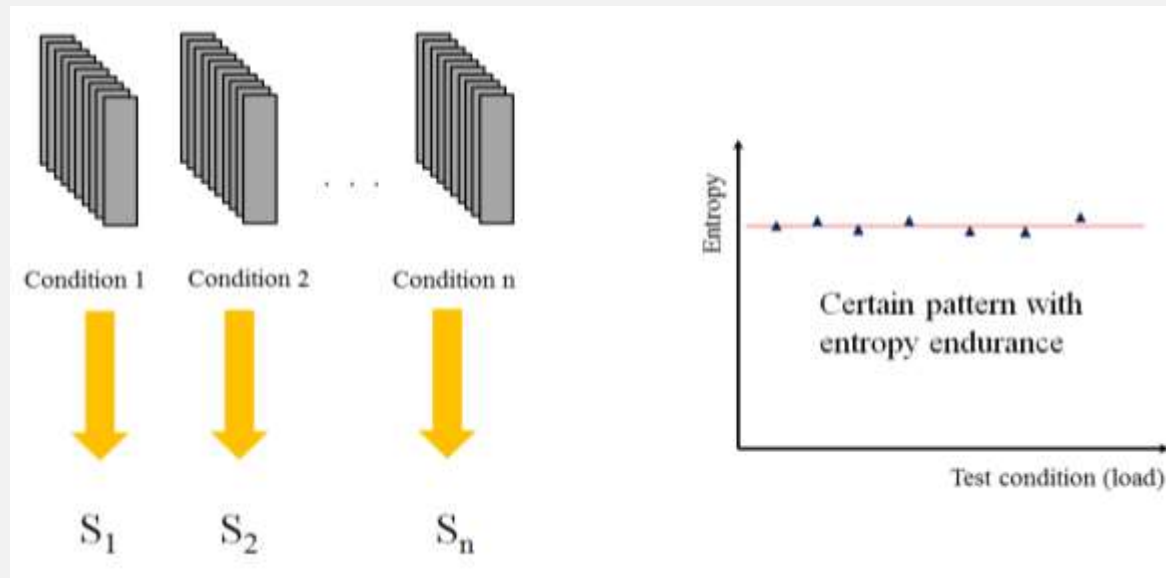
## Arranging Work Data by Making up Matching Table

- ✦ Collected forward / reverse work data at the cycle of every 0.01 % increment
- ✦ This process made up 10,000 by 20 tables of forward / reverse work

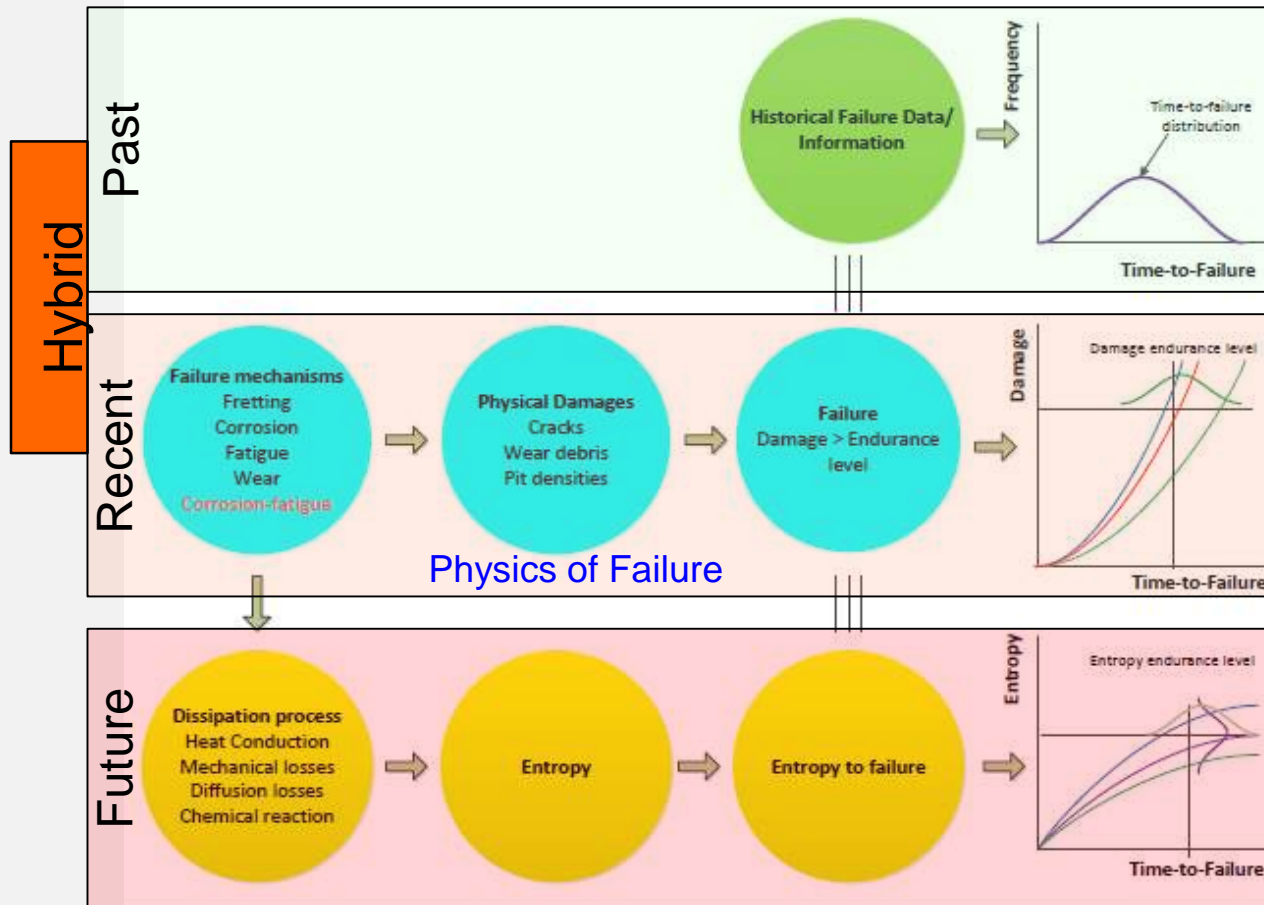


# Works to be done

- Crook's fluctuation theorem is developed in microscale. The validity of such theorem needs to be investigated in macroscale where the sources of fluctuations are different from microscale.
- Experiments needs to be performed in different experimental conditions to investigate the existence of the entropic limit.



# Thermodynamics as the Science of Reliability

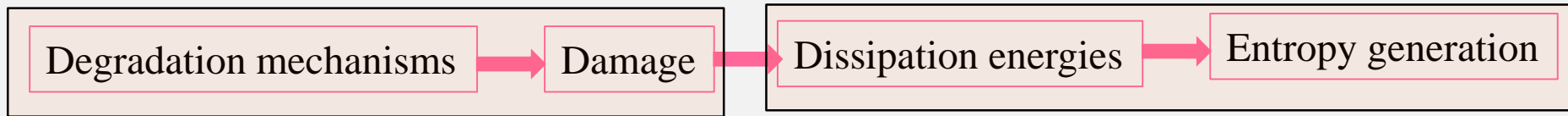


## Why Entropy?

- ✓ 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



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

An entropic theory follows<sup>[1]</sup>:

*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:  $D = \frac{\gamma_d - \gamma_{d0}}{\gamma_{dE} - \gamma_{d0}}$

Entropy generation,  $\gamma_d$ , monotonically increases starting at time zero from a theoretical value of zero or practically some initial entropy,  $\gamma_0$ , to an entropic-endurance value,  $\gamma_d$





# Total Entropy

- The variation of *total entropy*,  $dS$ , is in the form of:  $dS = d^r S + d^d S$ .

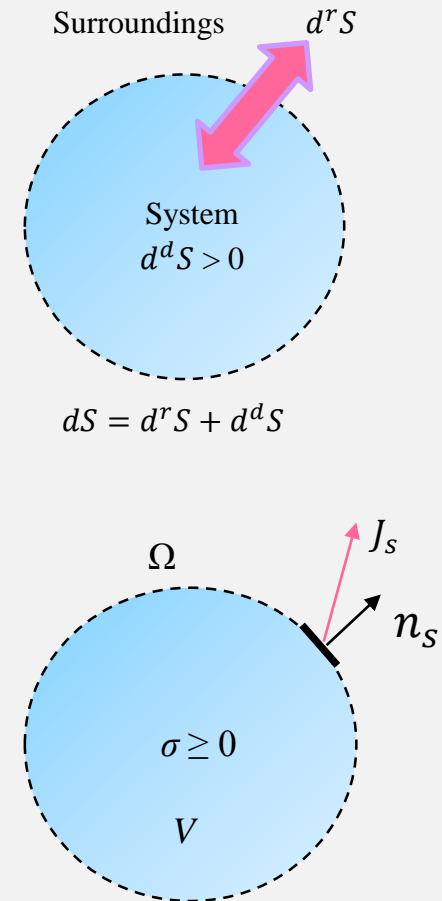
$d^r S$  = exchange part of the entropy supplied to the system by its surroundings through transfer of matters and heat:

$$\frac{d^r S}{dt} = - \int^{\Omega} \mathbf{J}_s \cdot \mathbf{n}_s dA$$

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

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

$J$ =entropy flux;  $\sigma$ =entropy generation/unit volume/unit time



# Total Entropy Generated

- Entropy generation  $\sigma$  involves a thermodynamic **force**,  $X_i$ , and an entropy **flux**,  $J_i$  as:

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

For near equilibrium condition interactions between multiple dissipation processes is captured by the **Onsager 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 |
|----------------|------------------|----------------------------|

$$\sigma = \frac{1}{T^2} \mathbf{J}_q \cdot \nabla T + \sum_{k=1}^n \mathbf{J}_k \left( \nabla \frac{\mu_k}{T} \right) + \frac{1}{T} \boldsymbol{\tau} : \boldsymbol{\epsilon}_p + \underbrace{\frac{1}{T} \sum_{j=1}^r v_j A_j}_{\text{Chemical reaction energy}} + \underbrace{\frac{1}{T} \sum_{m=1}^h c_m \mathbf{J}_m (-\nabla \psi)}_{\text{External fields energy}}$$

|                          |                        |
|--------------------------|------------------------|
| Chemical reaction energy | External fields energy |
|--------------------------|------------------------|

$J_n$  ( $n = q, k, \text{ and } m$ ) = thermodynamic fluxes due to heat conduction, diffusion and external fields,  $T$ =temperature,  $\mu_k$  = chemical potential,  $v_i$ =chemical reaction rate,  $\boldsymbol{\tau}$  =stress tensor,  $\boldsymbol{\epsilon}_p$  =the plastic strain rate,  $A_j$  =the chemical affinity or chemical reaction potential difference,  $\psi$  =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," 3<sup>rd</sup> edition; Cambridge University Press: Cambridge, UK, 2000.



# Examples of Force and Flux of Dissipative Processes

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

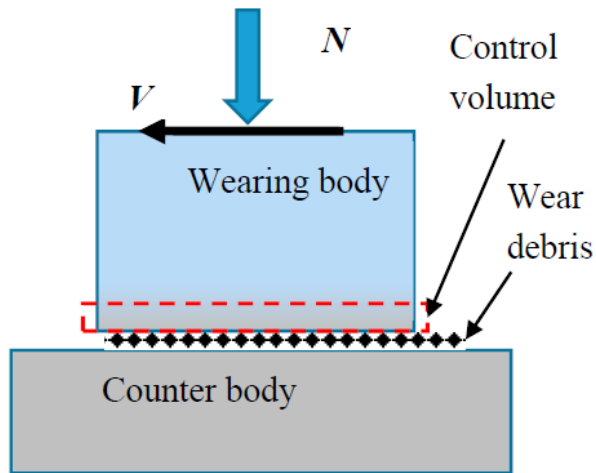
| Primary mechanism             | Thermodynamic force, $X$                                     | Thermodynamic flow, $J$                               | Examples of materials damage process |
|-------------------------------|--|---|--------------------------------------|
| Heat conduction               | Temperature gradient, $\nabla(1/T)$                          | Heat flux, $\mathbf{q}$                               | Fatigue, creep, wear                 |
| Plastic deformation of solids | Stress, $\sigma/T$   | Plastic strain, $\dot{\epsilon}_p$                    | 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, $\mathbf{J}_k$                        | 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 $(\tilde{\sigma} - \omega \mathbf{I})/T$ | Creep deformation rate, $\mathbf{R}$                  | Creep                                |

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

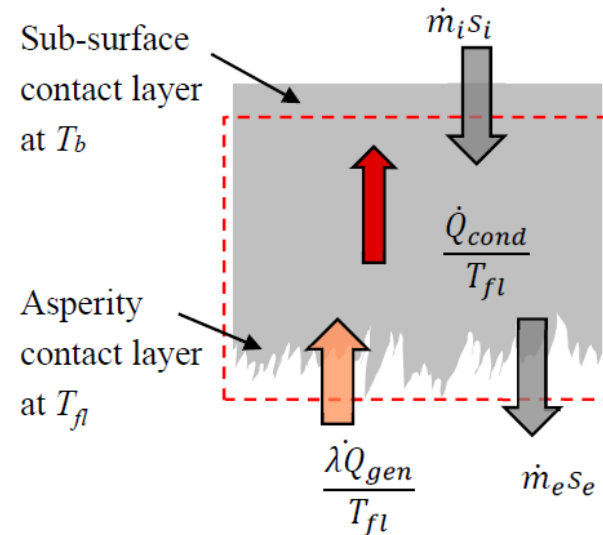


# Entropic approach to wear damage

Schematic of a tribosystem (a) including wearing body and counter body, (b) control volume enclosing interface of dissipative processes, thermodynamic model.



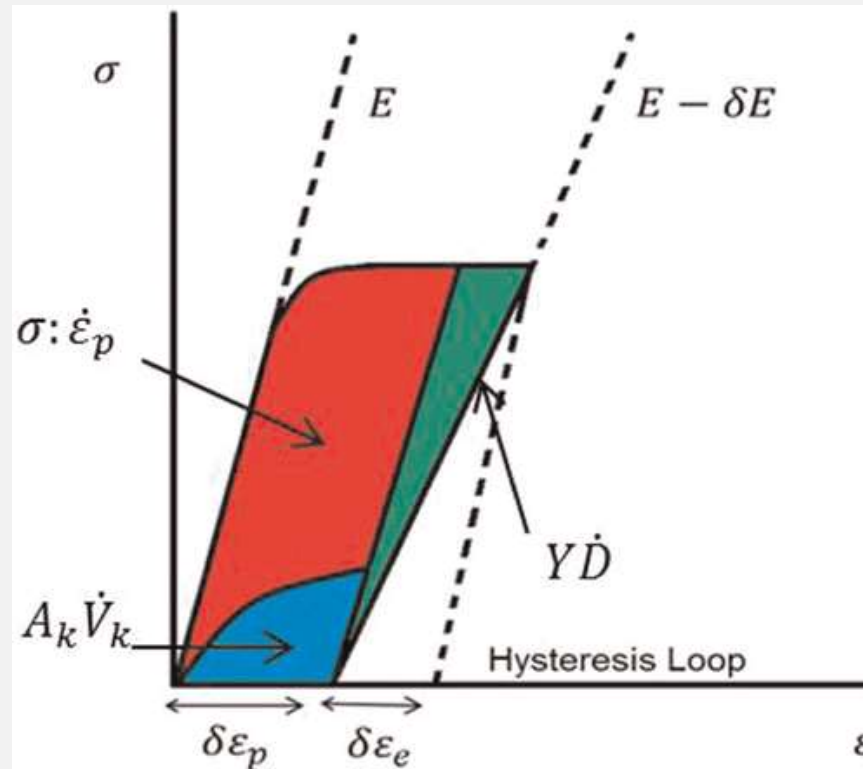
(a)



(b)

Amiri, Mehdi, and Mohammad Modarres. "An entropy-based damage characterization." *Entropy* 16.12 (2014): 6434-6463.

# Entropic approach to Low cycle fatigue of metals



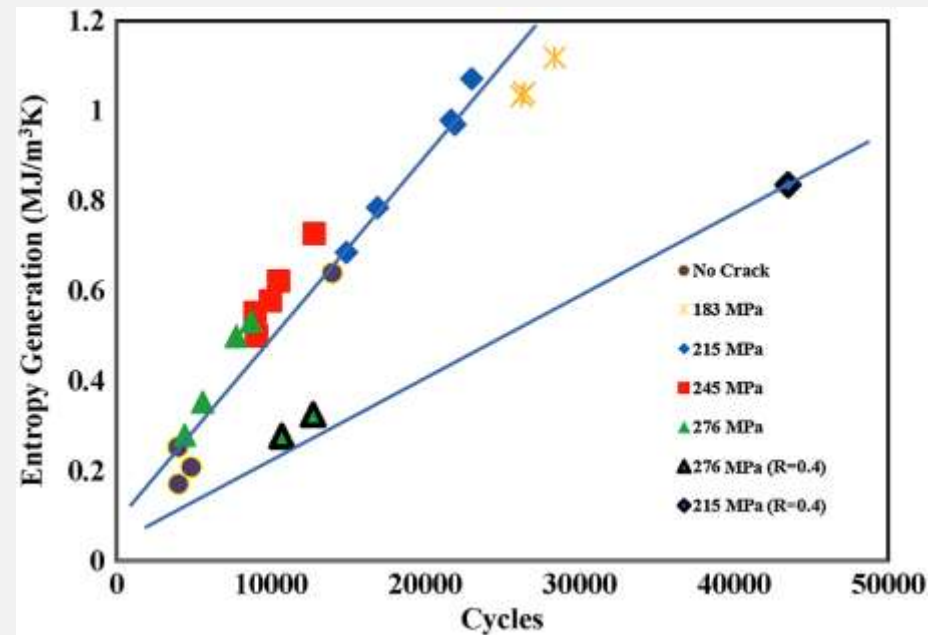
Hysteresis energy

Ontiveros, V. L., Modarres, M., & Amiri, M. (2015). Estimation of reliability of structures subject to fatigue loading using plastic strain energy and thermodynamic entropy generation. Proceedings of the Institution of Mechanical Engineers, Part O: Journal of Risk and Reliability, 229(3), 220-236.

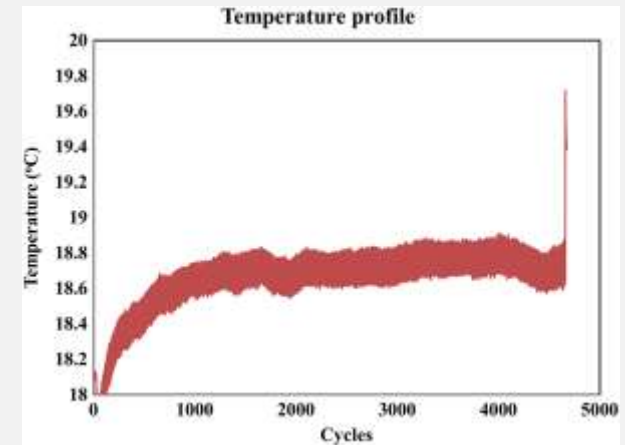


# Entropic approach to low cycle fatigue of metals

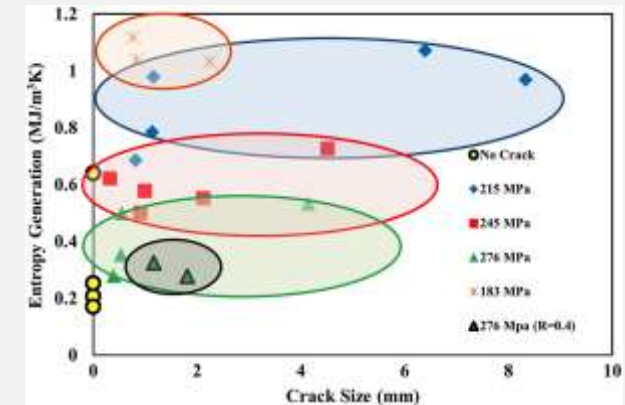
$$\sigma = \frac{1}{T} \tau : \dot{\epsilon}_p \quad \text{Plastic deformation entropy}$$



Entropy generation at crack initiation.



Example of a specimen temperature evolution.

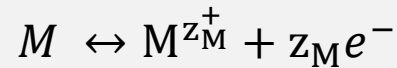


Entropy generation for various crack sizes.

Ontiveros, V., Amiri, M., Kahirdeh, A., & Modarres, M. (2016). Thermodynamic entropy generation in the course of the fatigue crack initiation. *Fatigue & Fracture of Engineering Materials & Structures*.

# Entropic-Based Damage from Corrosion-Fatigue (CF)

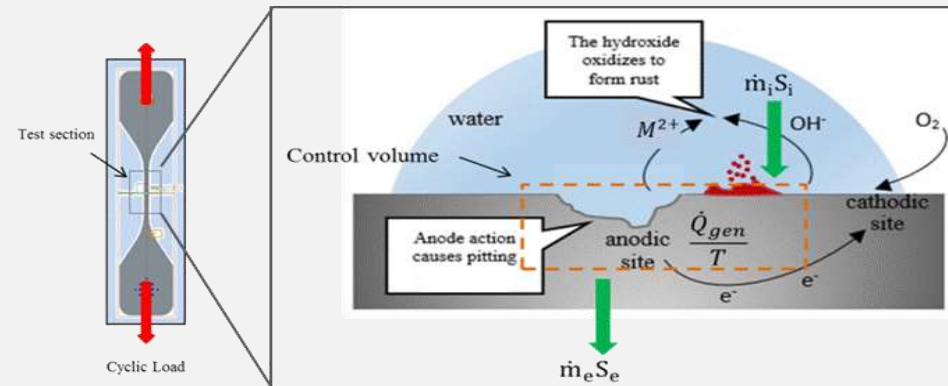
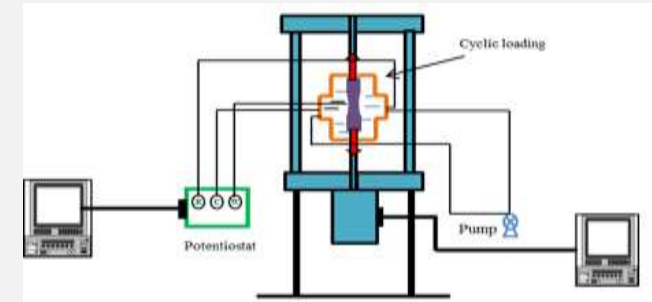
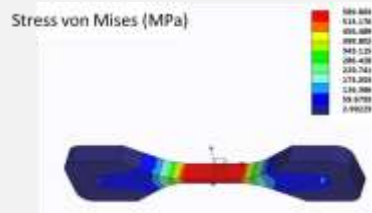
- Oxidation and reduction reactions of metallic electrode,  $M$ , under CF:



$O$  = 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

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

Diffusion  
dissipations

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

Chemical reaction  
dissipations

Mechanical  
dissipations

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

Hydrogen  
embrittlement  
dissipation

$$+ \sigma_H$$

$T$  = 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 reduction reaction,  $E_{M_{conc,c}}$  and  $E_{O_{conc,c}}$  = concentration over-potentials for the cathodic oxidation and cathodic reduction reactions,  $\alpha_M$  and  $\alpha_O$  = 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,  $\boldsymbol{\tau}$  = plastic stress,  $\dot{D}$  = dimensionless damage flux,  $Y$  the elastic energy, and  $\sigma_H$  = entropy generation due to hydrogen embrittlement.

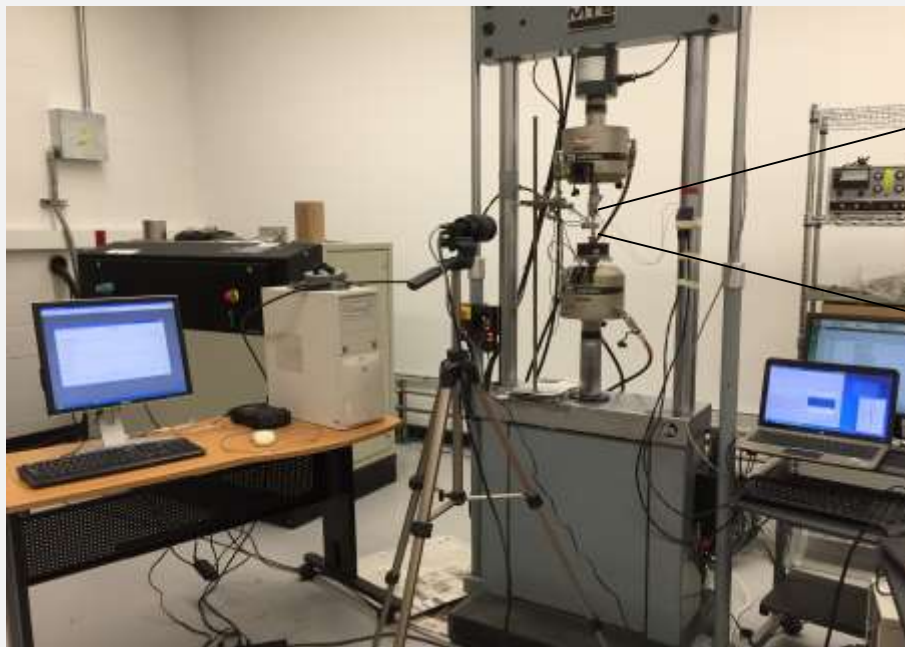




# Corrosion Fatigue (CF) Experimental Set up

- 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

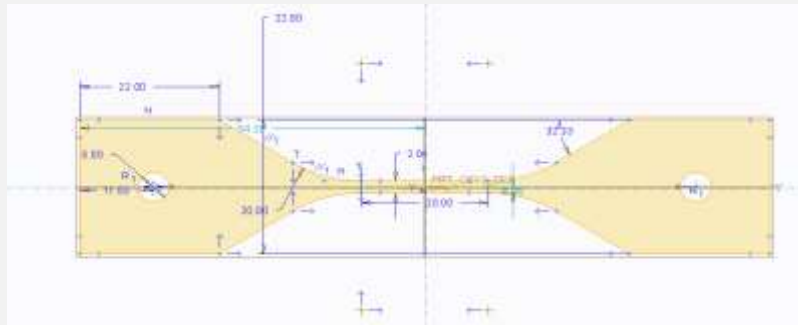
CF tests done while measuring the open circuit potential (OCP) vs. reference electrode during load-unload



Electrochemical corrosion cell made of plexiglass

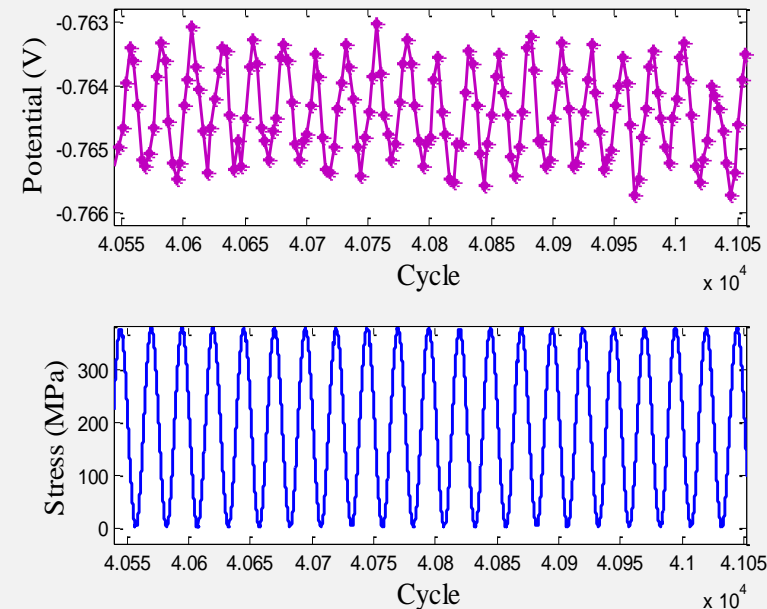


# CF Test Procedures



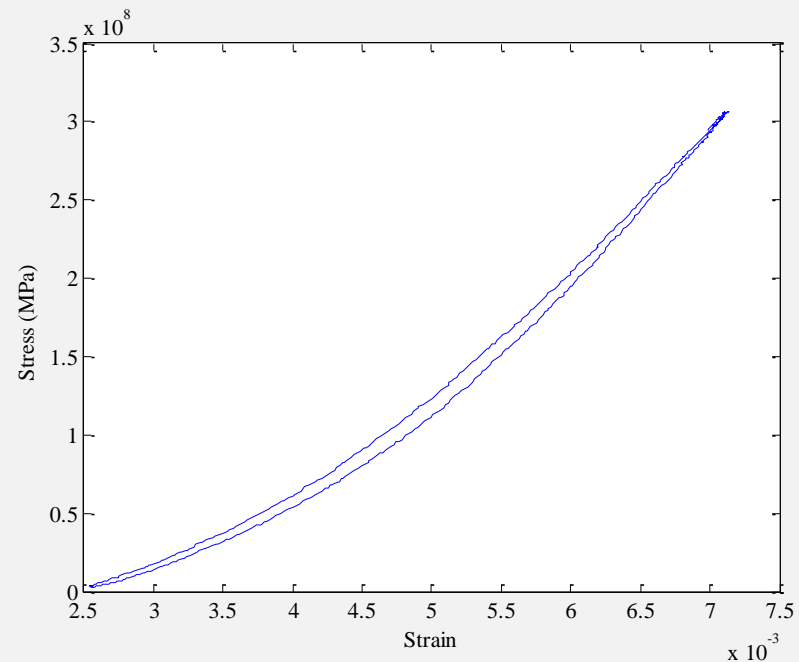
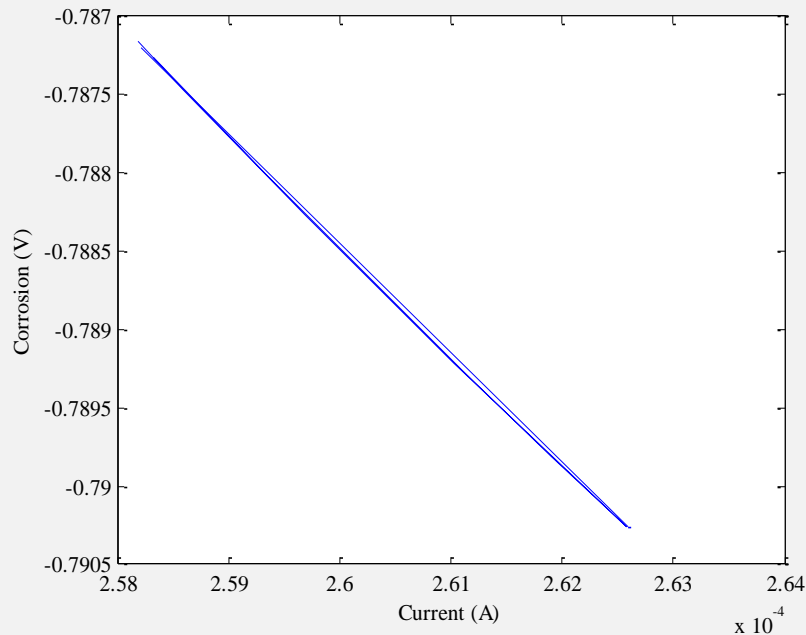
## Forces and fluxes were measured under CF

- 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



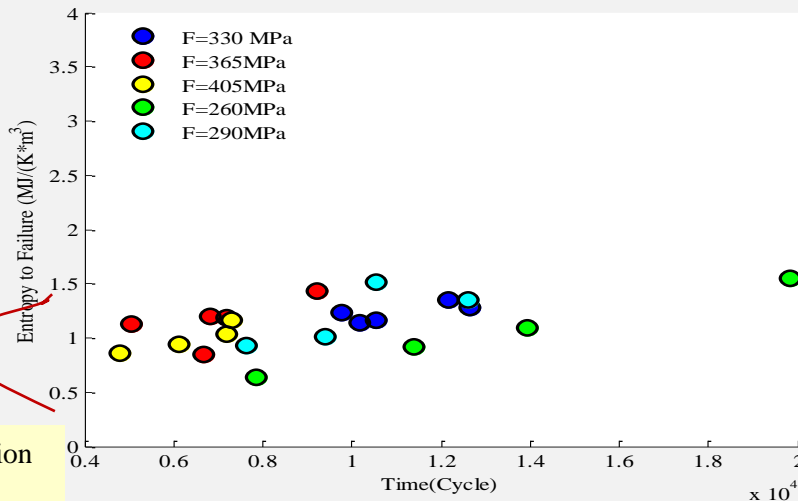
# Entropy Generation in CF

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

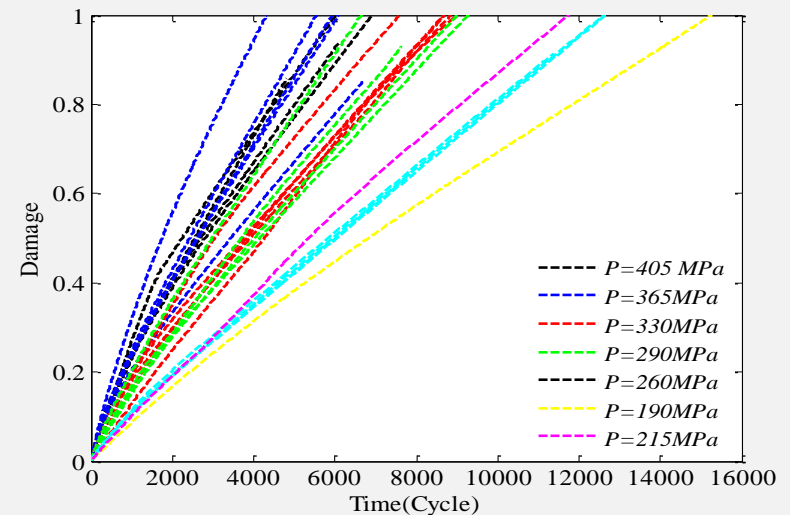


# Entropic Endurance and Entropy-to-Failure

- 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

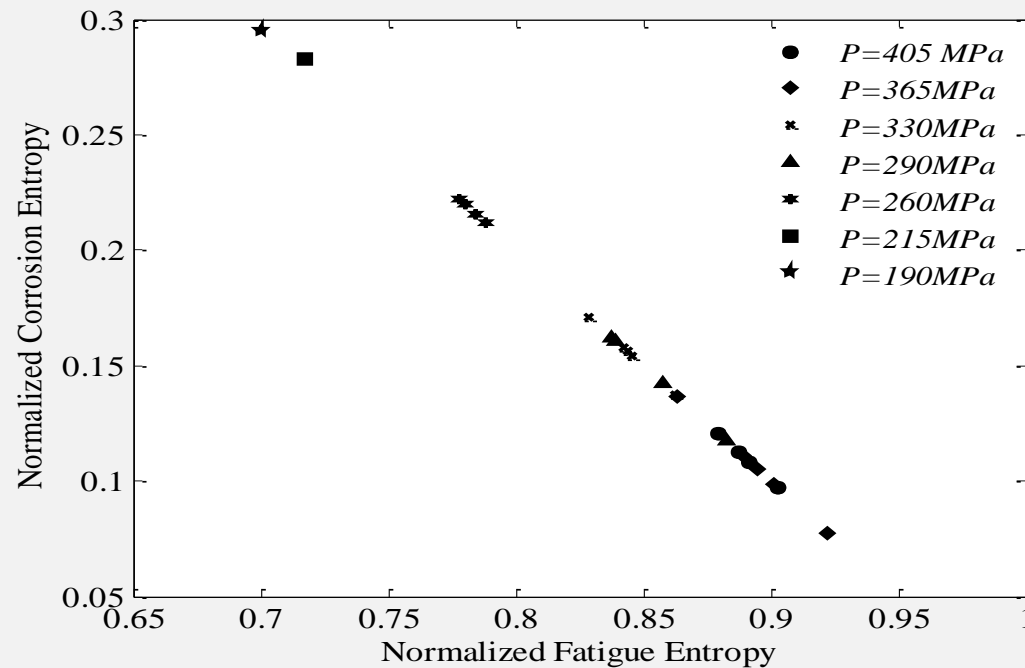


Distribution  
of  
entropic-  
endurance



# 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

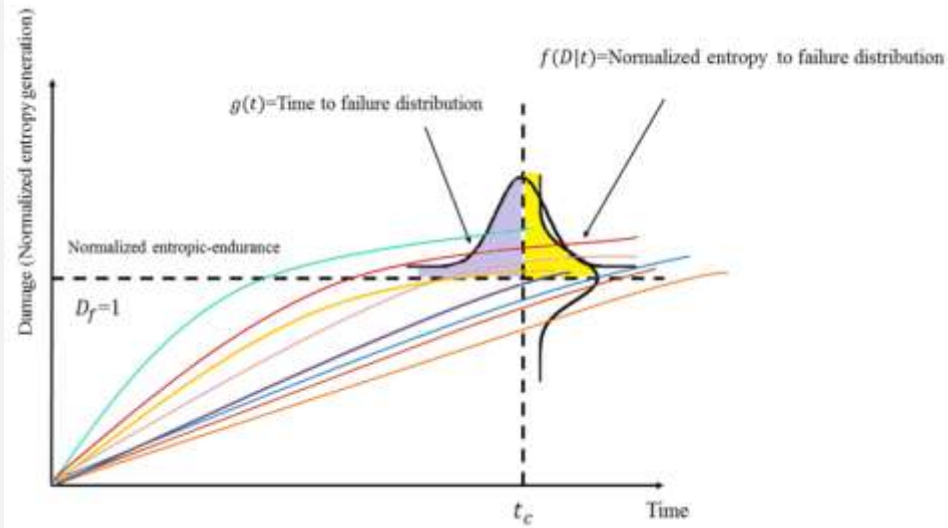
- Assuming a constant entropic-endurance,  $D_f$

- The reliability function can be expressed as [1]

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

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

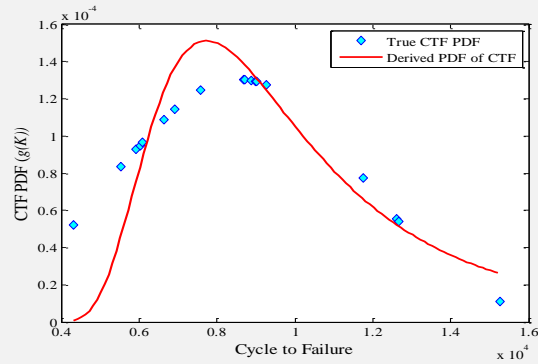
$T_c$ =Current operating time;  $g(t)$ =distribution of time-to-failure,  $f(D|t)$ = distribution of damage at  $t$



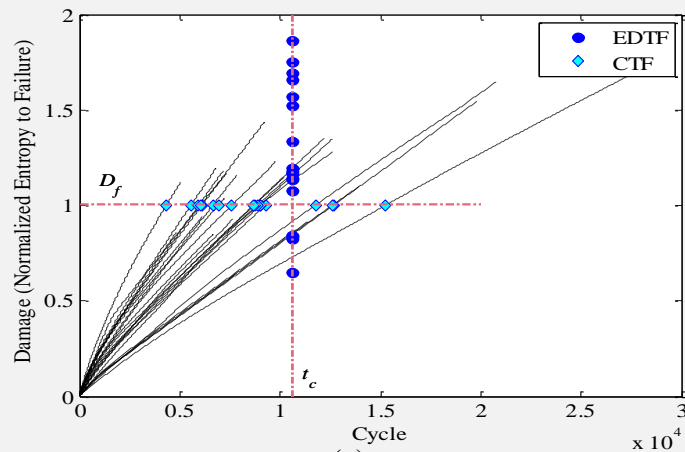
[1] Thermodynamics as a Fundamental Science of Reliability, A. Imanian, M. Modarres, Int. J. of Risk and Reliability, Vol.230(6), pp.598-608. DOI: 10.1177/1748006X16679578.(2016).



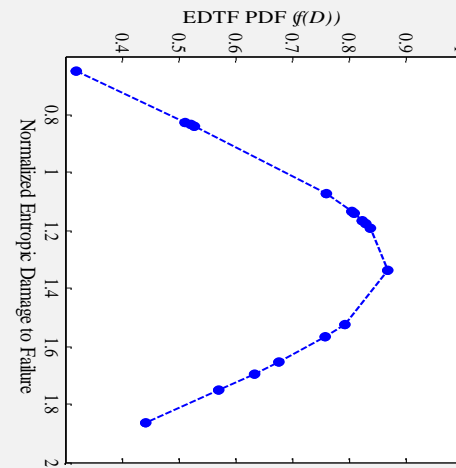
# Entropic-Based CF Reliability



(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



# 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)

