Entropy as an Indication of Damage in Engineering Materials

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Acknowledgments

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7. Prof. C. Wang (Corrosion/electrolysis consultant)
8. Prof. Enrique Droguett (Adjunct Associate Professor)
9. Prof. Mohammad Modarres (PI)

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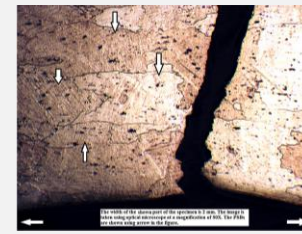
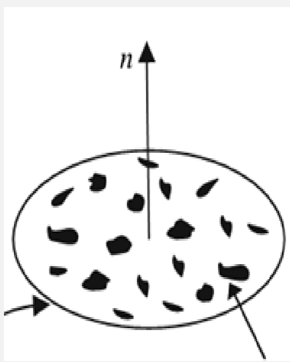
Objectives

- Describe damage resulted from failure mechanisms within entropic framework
- Understand sources of irreversible energy dissipation measurements in the fatigue process, i.e. mechanical, thermal, and acoustic
- Develop entropy for each dissipation measurement representing damage or state of current material based on thermodynamic, information, and statistical mechanics theorems
- 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)
  - ➢ 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

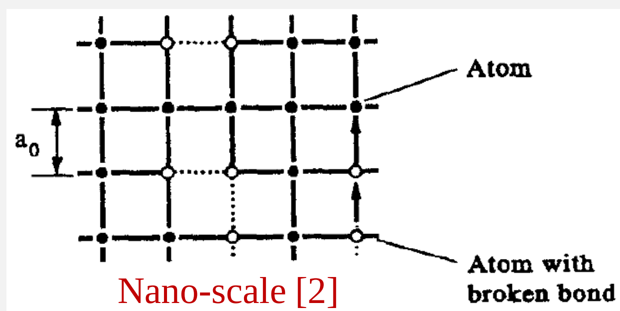




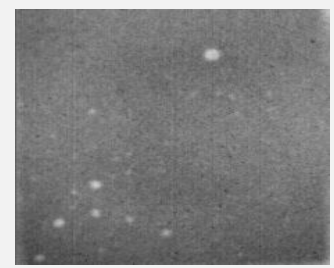
$$D(\boldsymbol{n}) = \frac{A_0 - A_e}{A_0}$$

Continuum damage mechanics [1]

Micro-scale



Nano-scale [2]

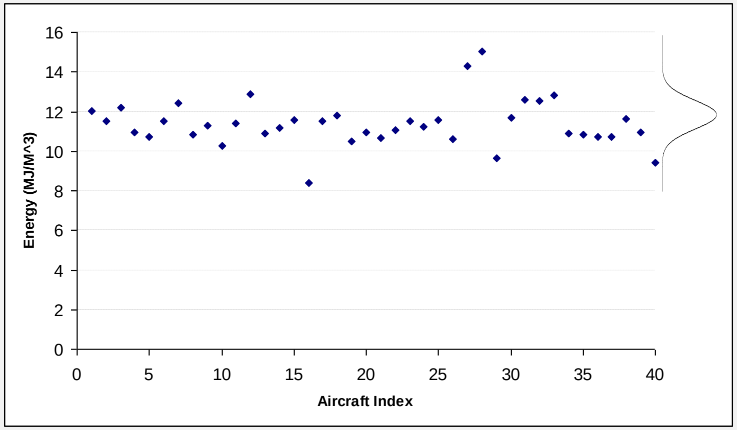


Meso-scale

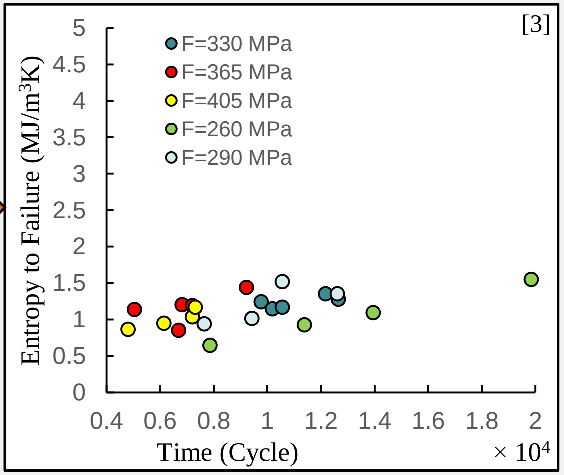
[1] J. Lemaitre, "*A Course on Damage Mechanics*", Springer, France, 1996.
[2] C. Woo & D. Li, "*A Universal Physically Consistent Definition of Material Damage",* Int. J. Solids Structure, V30, 1993

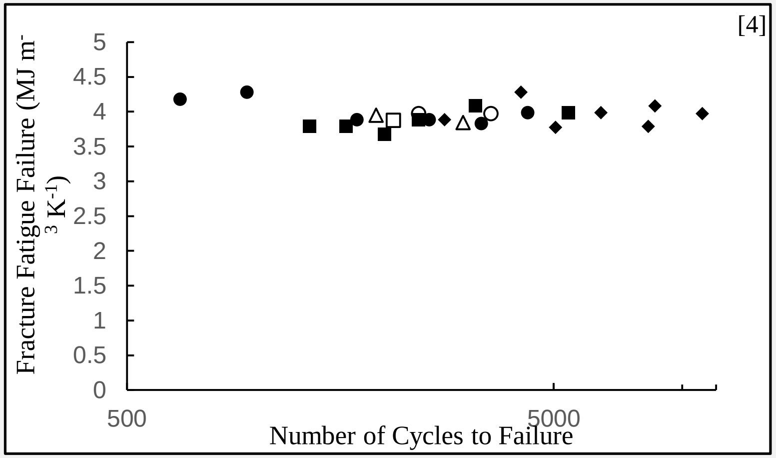
Motivation (Cont.)

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



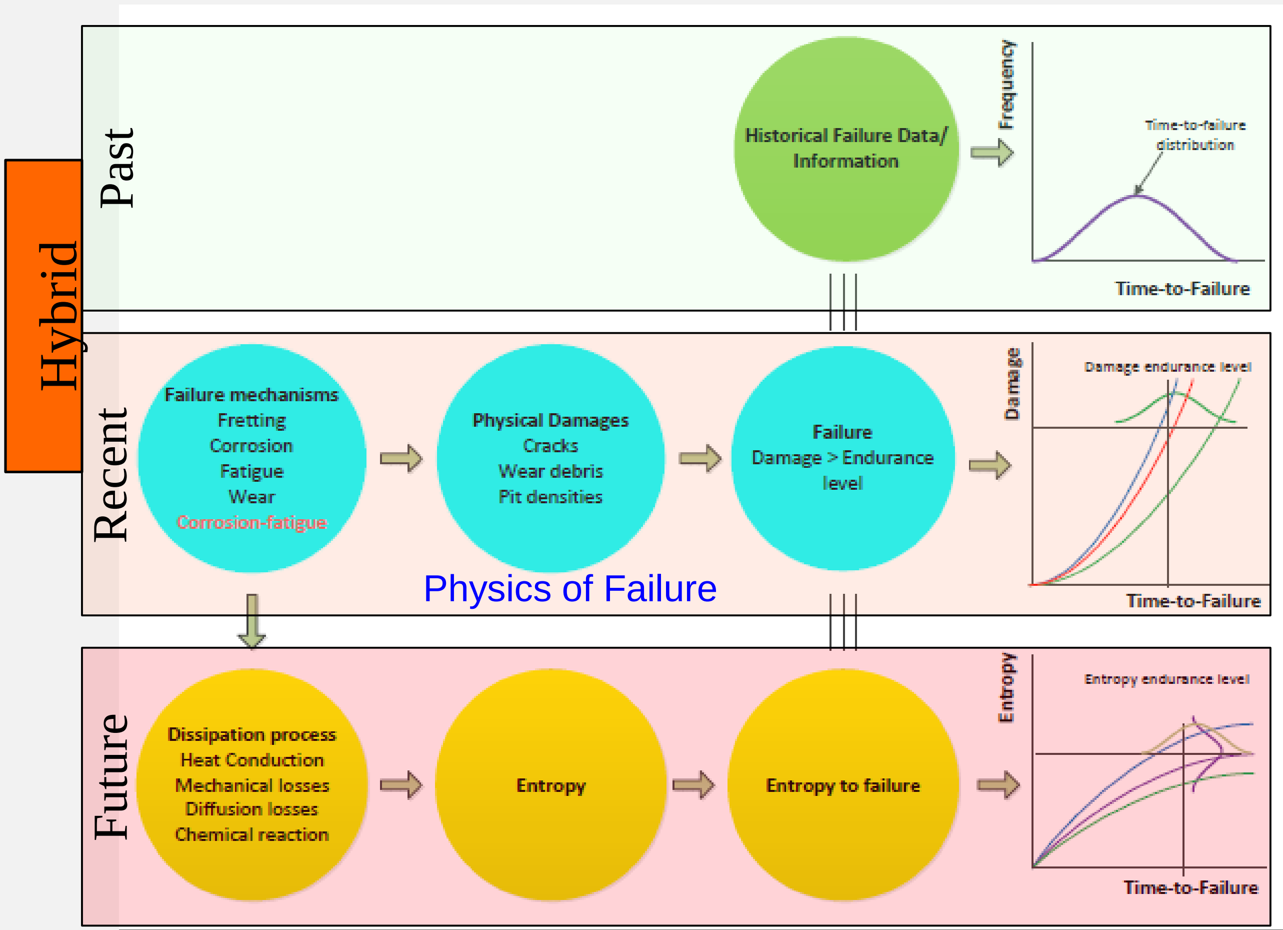


Entropy to Fracture

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

[4] 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

Entropy 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[3]:

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

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

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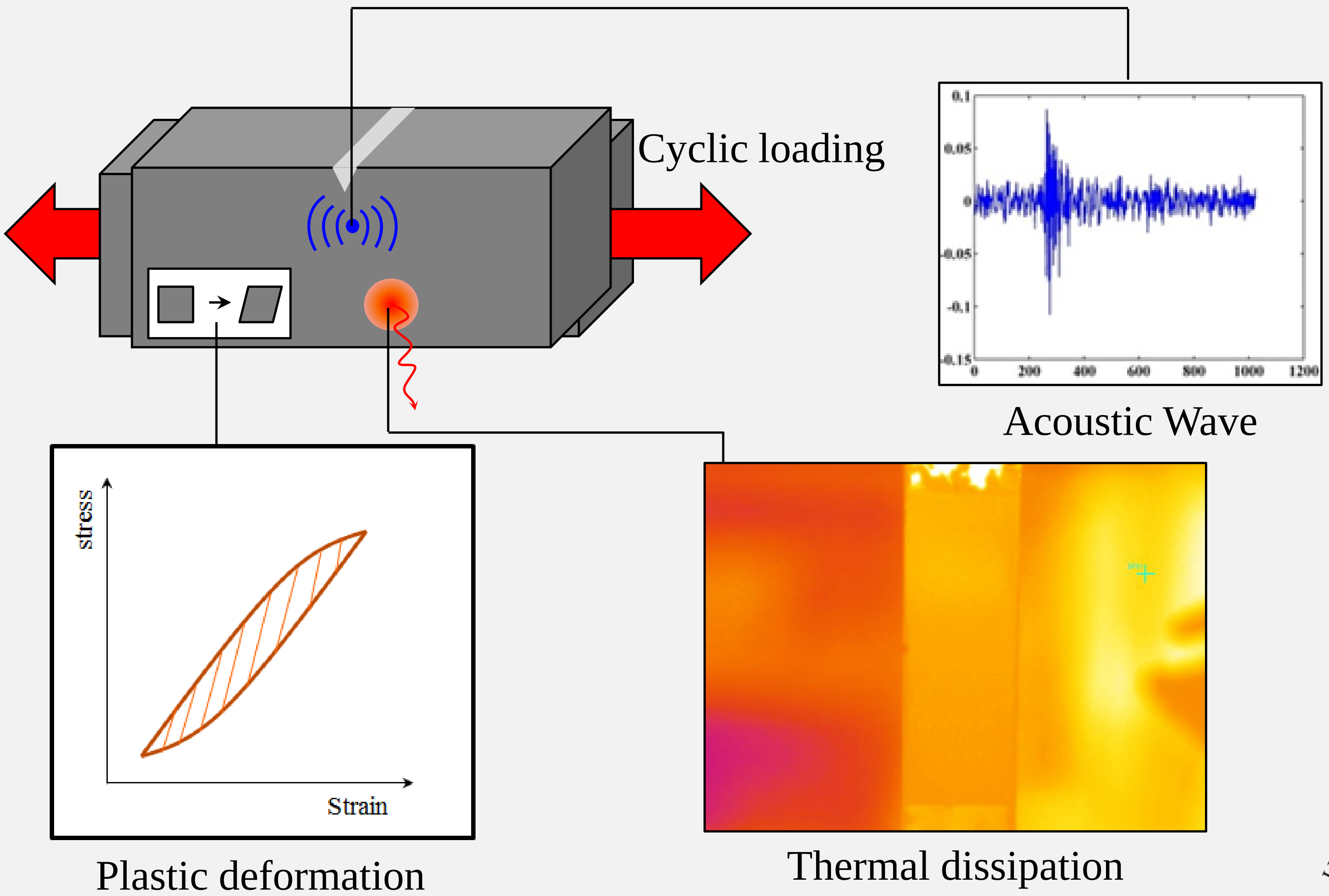
Sources of Dissipation in Fatigue Process



[5] Ali Kahirdeh and M.M. Khonsari, Energy dissipation in the course of the fatigue degradation: Mathematical derivation and experimental quantification, International Journal of Solids and Structures 77 (2015): 74-85

Entropic Approaches in Fatigue Process

Dissipation (Measurement) Source	Entropic Approach	Related Equation
Plastic Deformation	Second Law of Thermodynamics	$\sigma = \frac{1}{T^2} \boldsymbol{J}_q . \nabla T - \Sigma_{k=1}^{n} \boldsymbol{J}_k \left(\nabla \frac{\mu_k}{T} \right) + \frac{1}{T} \boldsymbol{\tau} : \dot{\boldsymbol{\epsilon}}_p + \frac{1}{T} \Sigma_{j=1}^{r} v_j A_j + \frac{1}{T} \Sigma_{m=1}^{h} c_m \boldsymbol{J}_m (-\nabla \psi)$
Thermal	Information Theory (Shannon)	$S = -\sum p_i \log p_i$
Acoustic Emission	Statistical Mechanics (Crooks)	$D(P_F \vert\vert P_R) = \sum P_{F,i} \ln \frac{P_{F,i}}{P_{R,i}}$

Entropy in Thermodynamics

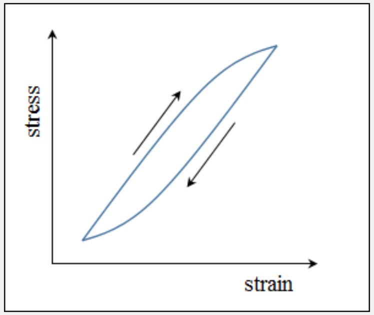
- Entropy generation σ involves a thermodynamic force, X_i, and an entropy flux, J_i as:

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

- Entropy generation of important dissipation phenomena leading to damage:

$$\sigma = \underbrace{\frac{1}{T^2}\boldsymbol{J}_q.\nabla T}_{\text{Thermal}} + \underbrace{\Sigma_{k=1}^{n}\boldsymbol{J}_k\left(\nabla\frac{\mu_k}{T}\right)}_{\text{Diffusion}} + \underbrace{\frac{1}{T}\boldsymbol{\tau}:\dot{\boldsymbol{\epsilon}}_p}_{\text{Plastic deformation}} + \underbrace{\frac{1}{T}\Sigma_{j=1}^{r} v_j\, A_j}_{\text{Chemical reaction}} + \underbrace{\frac{1}{T}\Sigma_{m=1}^{h} c_m \boldsymbol{J}_m(-\nabla\psi)}_{\text{External fields}}$$

$\boldsymbol{J}_n$ $(n = q, k, \text{and } m)$ = 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 *, **

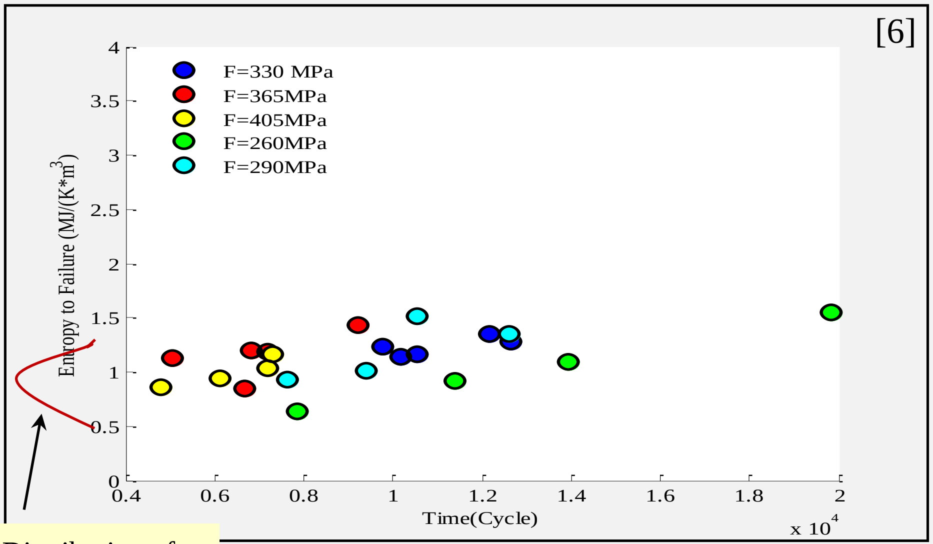


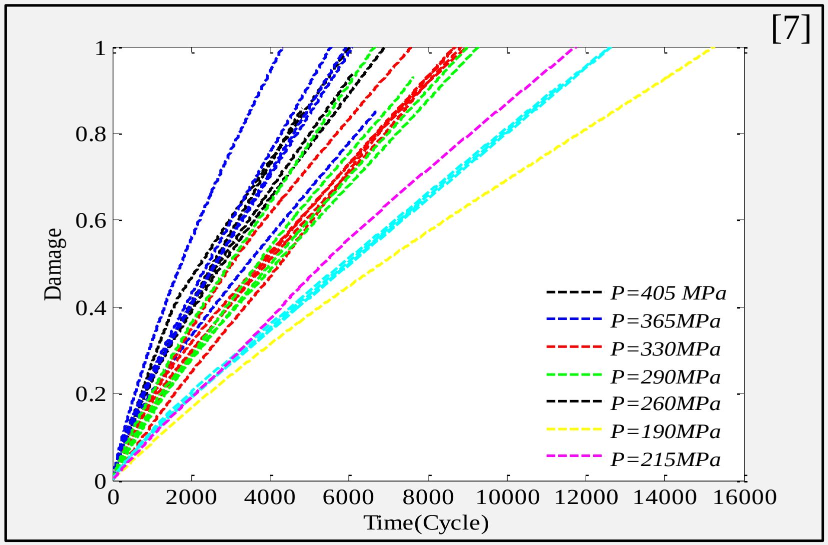
$$\Delta S_{total} = \frac{W^{diss}}{T} = \frac{Hysteresis\ Area}{T}$$

Hysteresis Area: From stress-strain analysis
T: From surface temperature measured by infrared camera or thermocouple

Entropy in Thermodynamics (Cont.)

- 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 future confirm the theory

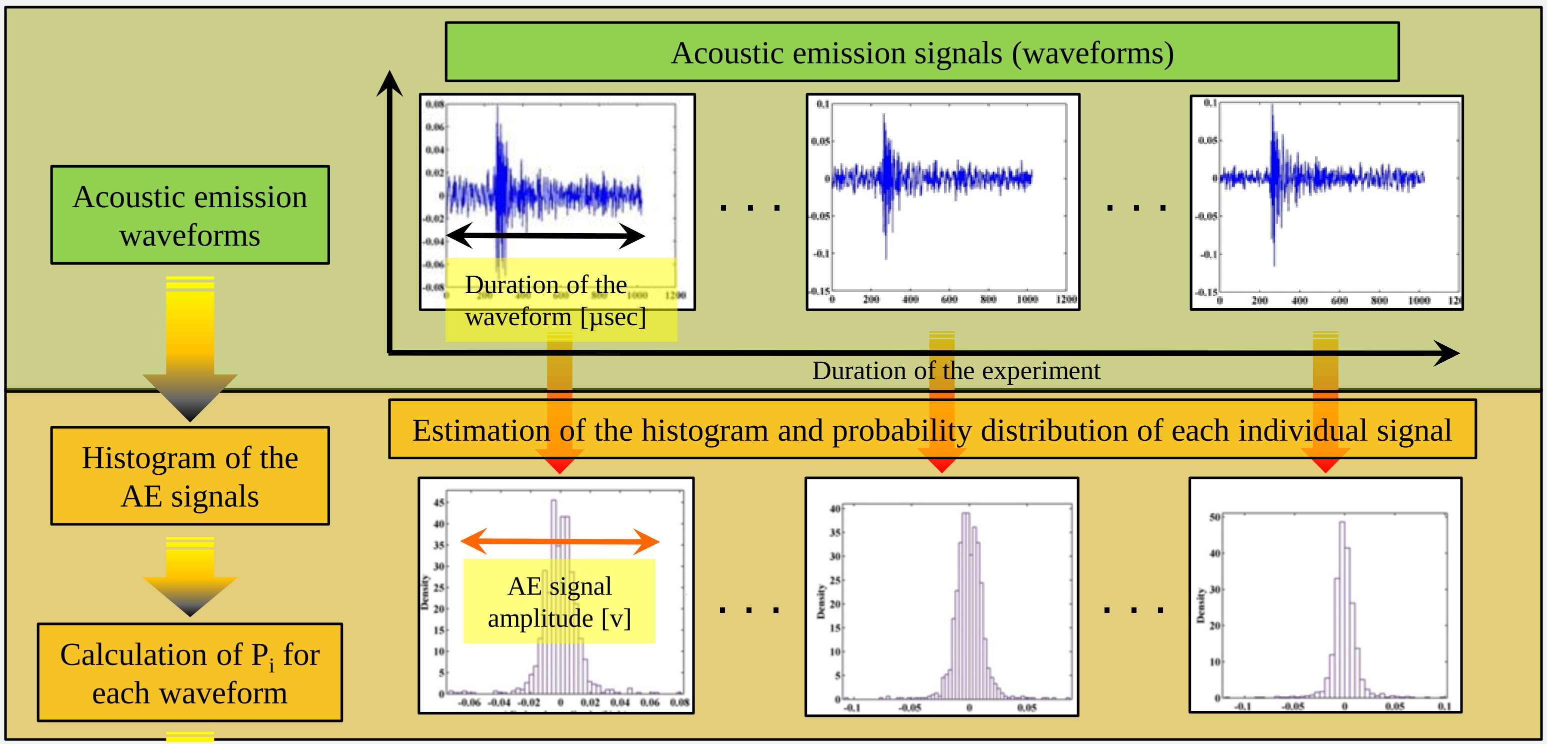


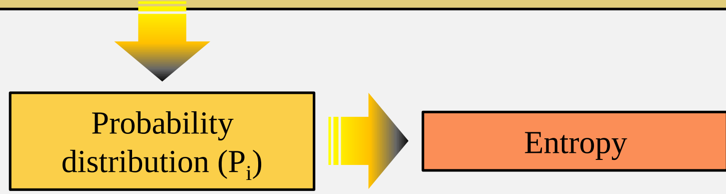


Distribution of entropic-endurance

[6] Mohammad Modarres, A General Entropic Framework of Damage: Theory and Applications to Corrosion-Fatigue, Structural Mechanics TIM 2015, 25-26 June 2015, Falls Church, VA, USA
[7] Anahita Imanian and Mohammad Modarres, Structural Health Monitoring, 2018, Vol. 17(2) 240-254

Entropy in Information Theory





$$S_I = \sum_{i=1}^{n} p_i \, log_2\left(\frac{1}{p_i}\right) = -\sum_{i=1}^{n} p_i \, log_2(p_i)$$

$$S_R = \int \rho \log \frac{\rho}{\rho_R} \, dx = \sum_{i=1}^{n} p_i \, log \, \frac{p_i}{p_{R,i}}$$

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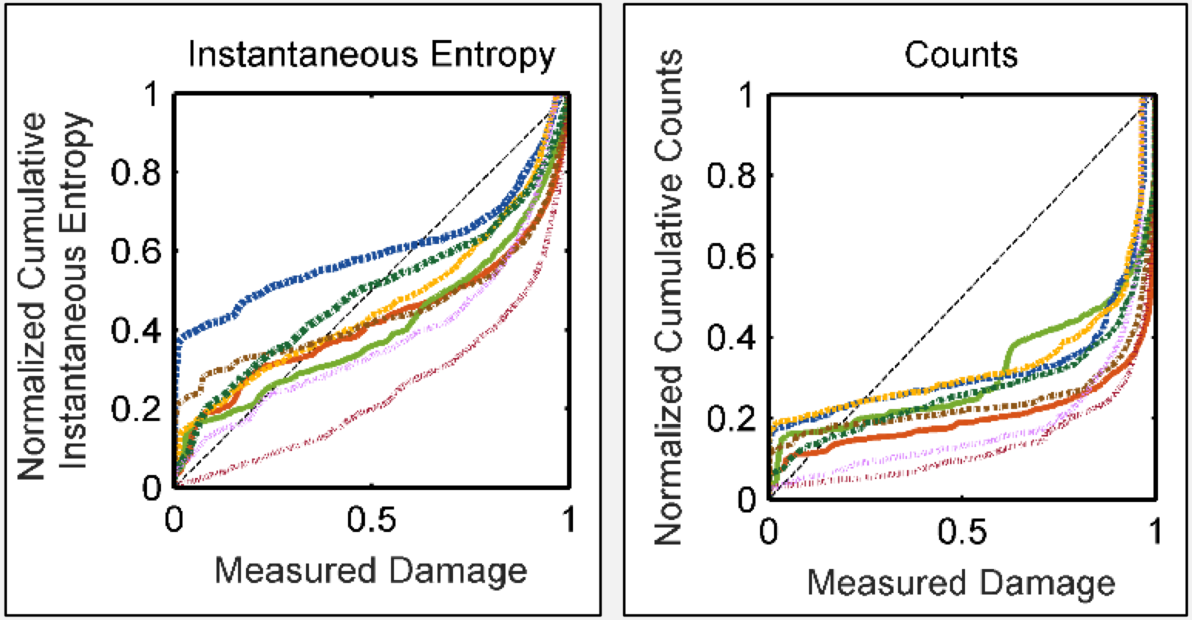
Entropy in Information Theory (Cont.)

- Cumulative AE information entropy correlated measured damage in elastic modulus
- Information entropy provided better correlation to damage compared with other AE features, e.g. counts



[8]

[8] Sauerbrunn, Christine M., et al. "Damage Assessment Using Information Entropy of Individual Acoustic Emission Waveforms during Cyclic Fatigue Loading." *Applied Sciences* 7.6 (2017): 562

Entropy in Statistical Mechanics

- Relative entropy (Kullback-Leibler divergence)

$$D(P_F||P_R) = \sum P_{F,i} \ln \frac{P_{F,i}}{P_{R,i}}$$

- In thermodynamics, relative entropy equals total entropy in forward process or reverse process

$$\begin{aligned} D(P_F||P_R) &= \beta\langle W\rangle_F - \beta\Delta F \\ &= \beta\langle W\rangle_F - \beta\Delta\langle E\rangle_F + \Delta S_F^{System} \\ &= -\beta\langle Q\rangle_F + \Delta S_F^{System} = \Delta S_F^{Total} \end{aligned}$$ [8]

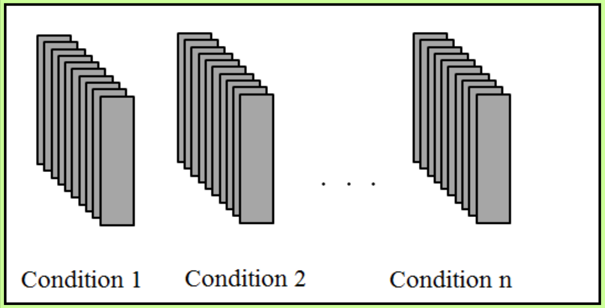
- For experimental proof, relative entropy is computed by repeating fatigue tests with same conditions and constructing forward / reverse work distributions

[8] Gavin E Crooks and David A Sivak, Measures of trajectory ensemble disparity in nonequilibrium statistical dynamics, Journal of Statistical Mechanics: Theory and Experiment, doi: 10.1088/1742-5468/2011/06/P06003

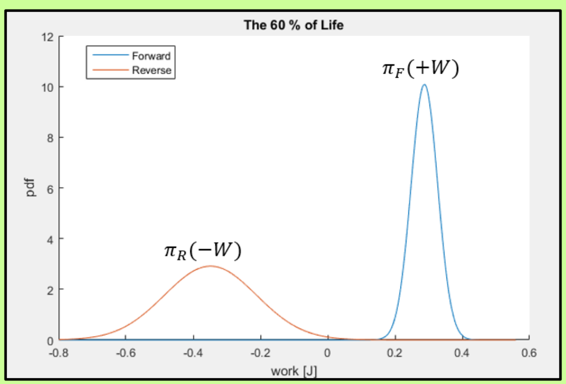
Entropy in Statistical Mechanics (Cont.)

- Analysis Procedure

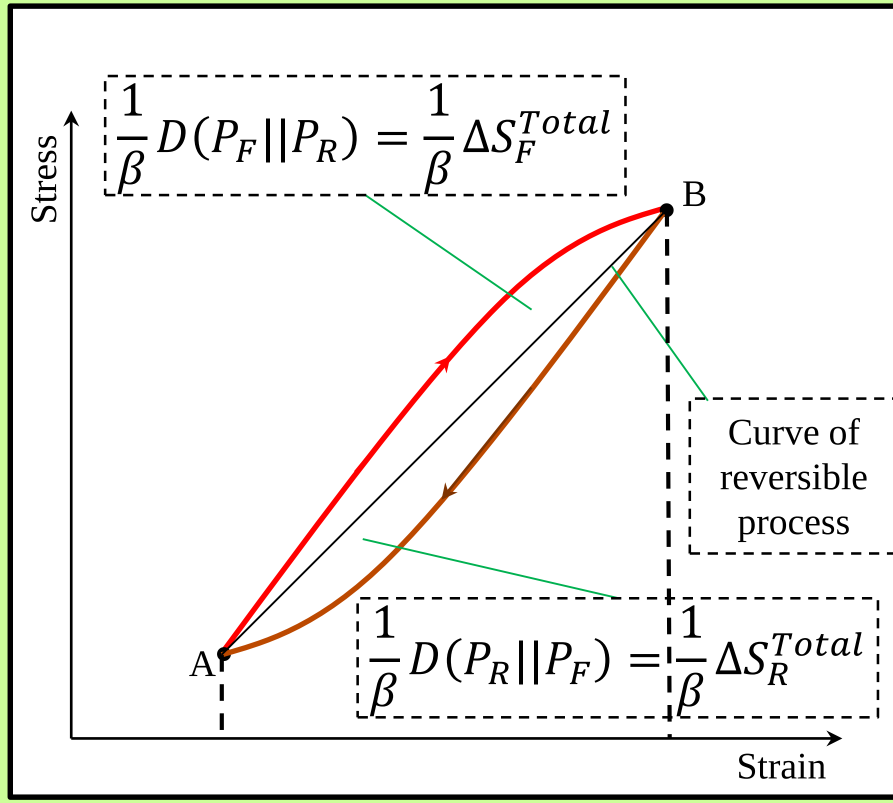
Multiple tests



Compose work distributions



Compute relative entropy



Fatigue Tests

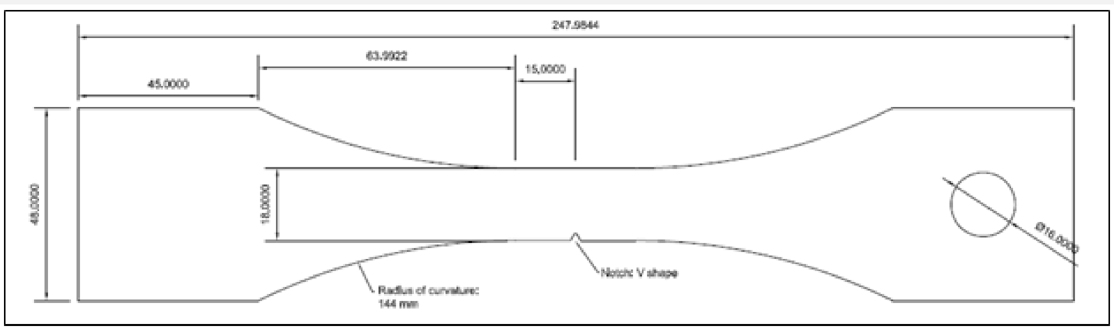
- Material and Specimen
  - Material: stainless steel 304L
  - Mechanical properties

σ_U [MPa]	σ_Y [MPa]	Elongation [%]	Hardness [RB]
613.8	320.3	54.06	85.00

  - Chemical composition [w%]

C	Cr	Cu	Mn	Mo	N	Ni	P	S	Si
0.0243	18.0595	0.3655	1.7720	0.2940	0.0713	8.0810	0.0300	0.0010	0.1930

  - Specimen: notched dogbone

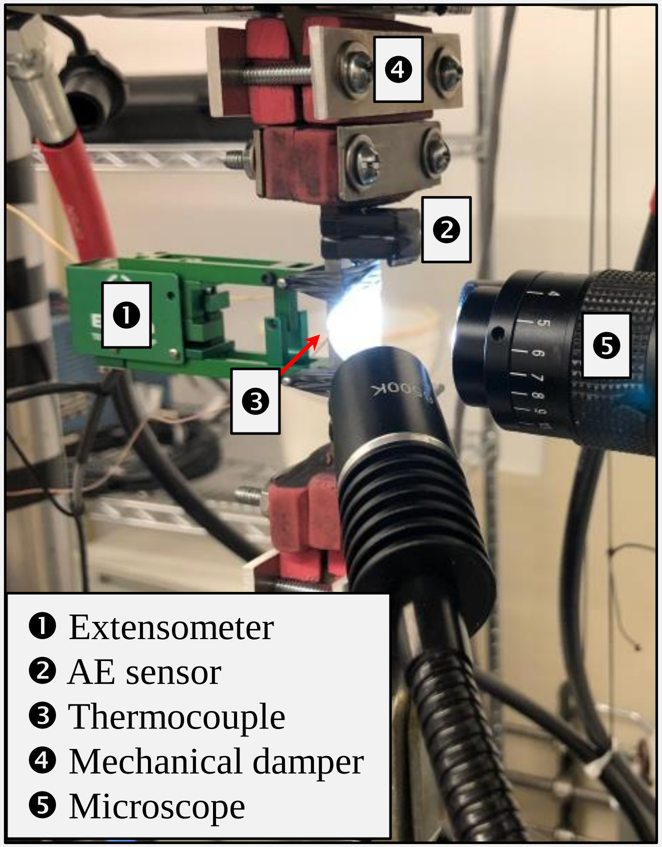


K_T at notch: 4.04

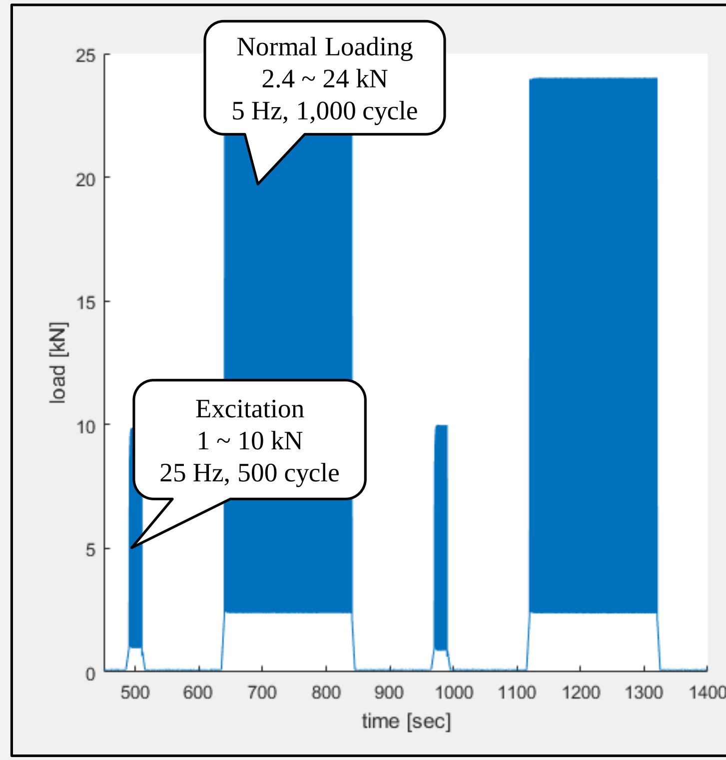
K_T at the hole: 3.44

Fatigue Tests (Cont.)

- Test Method
  - Measurements



  - Loading condition



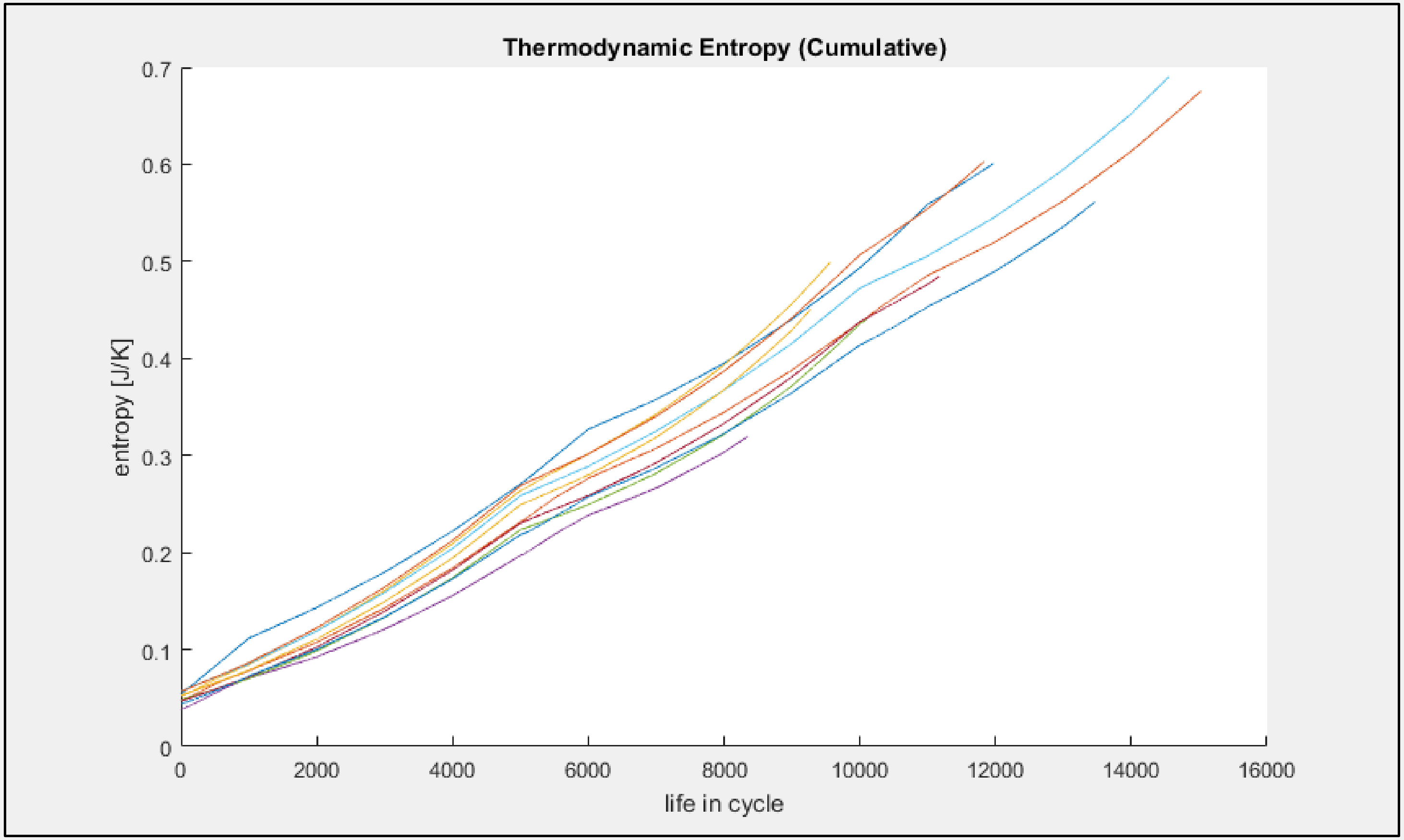
Test Results

- Test Summary

Test	Life at initiation	Life at .25 mm	Life at fracture
1	11,091	11,972	17,589
2	13,751	15,025	22,106
3	8,398	9,564	14,529
4	7,517	8,348	14,660
5	9,269	10,099	15,832
6	13,319	14,554	21,355
7	10,508	11,171	17,505
8	12,659	13,459	20,155
9	11,434	11,833	17,175
10	8,711	9,275	14,381
Average	8,888	9,608	14,607

Test Results (Cont.)

- Thermodynamic Entropy



Test Results (Cont.)

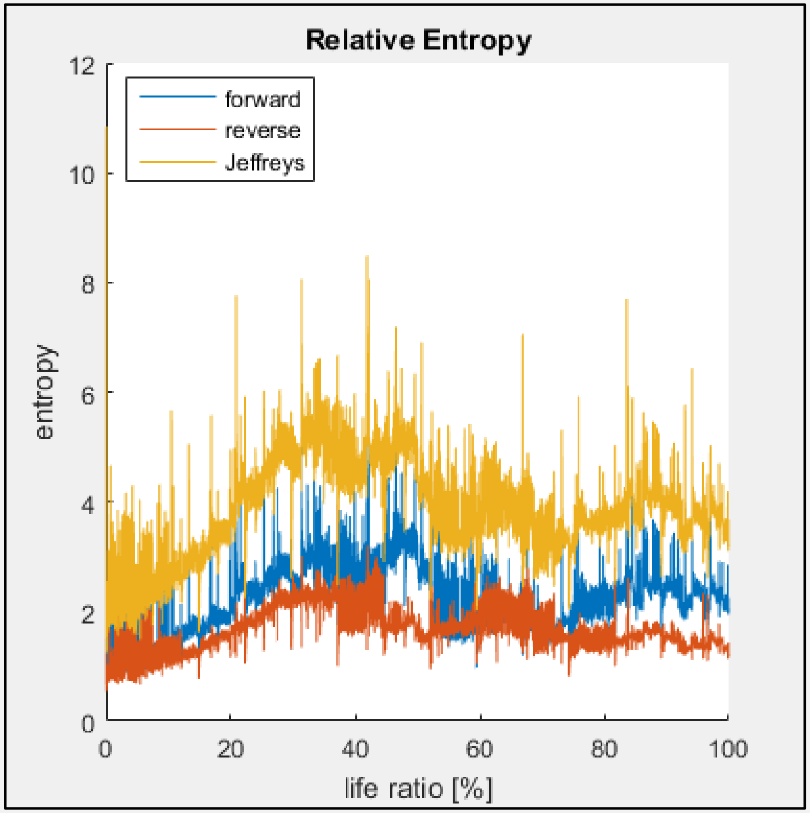
- AE Information Entropy (Ex: Test 1)

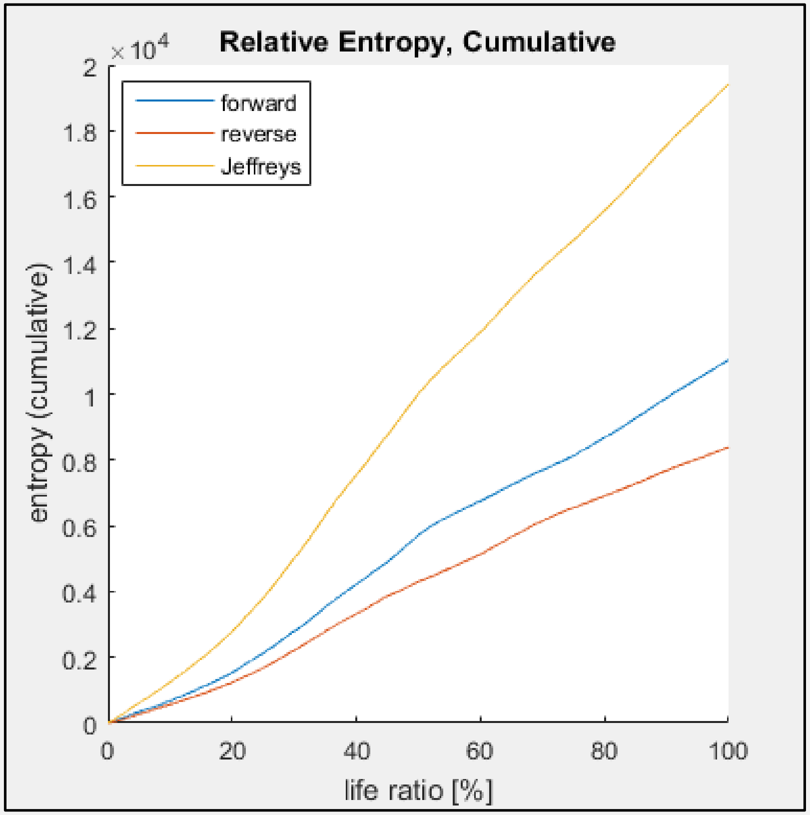
Test Results (Cont.)

- AE Relative Entropy (Ex.: Test 1)

Test Results (Cont.)

- Relative Entropy in Statistical Mechanics





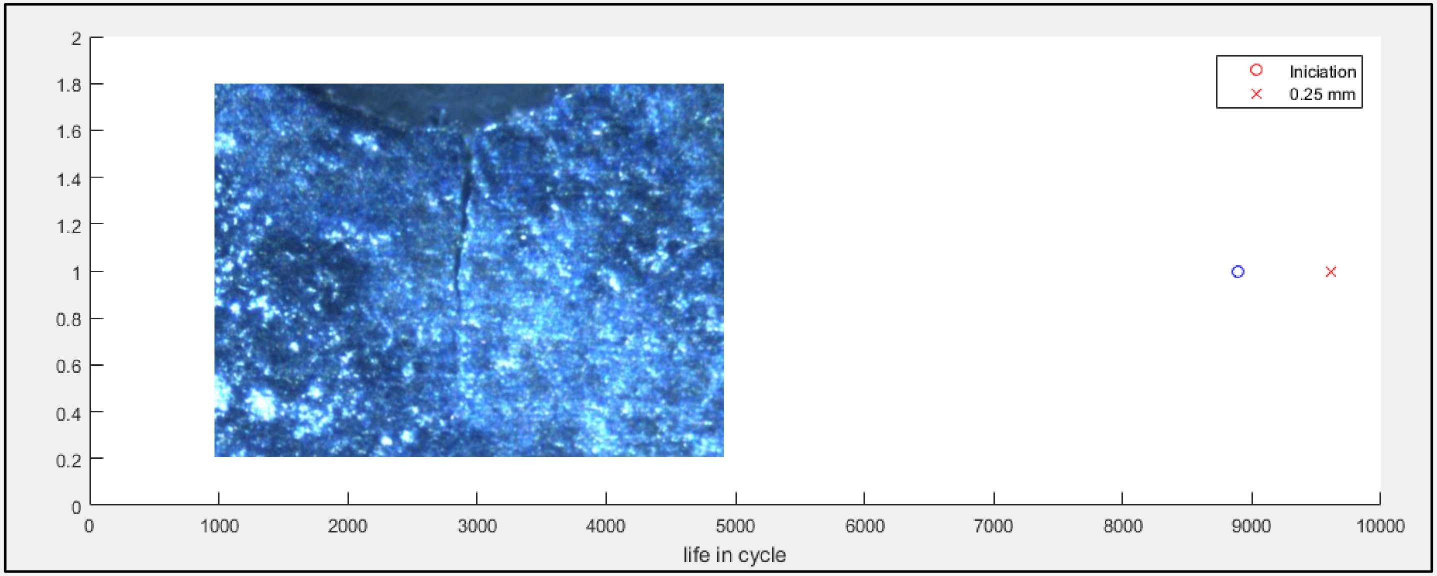
Conclusions

- Three different approaches to derive the entropic damage were investigated: classical thermodynamics, statistical mechanics and information theory
- A thermodynamic theory of damage proposed and tested
- Damage model derived from 2nd law of thermodynamics and used to develop models for reliability of structures
- The theory was verified through corrosion-fatigue tests
- The proposed theory offered a more fundamental model of damage and allowed incorporation of all interacting dissipative processes
- Statistical mechanics-based entropic damage theory was proposed
- Additional tests and verifications would be needed

Thank you

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)
  - 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



Entropy in Thermodynamics

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

Mechanical dissipations

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

$$+ \sigma_H$$

Hydrogen embrittlement dissipation

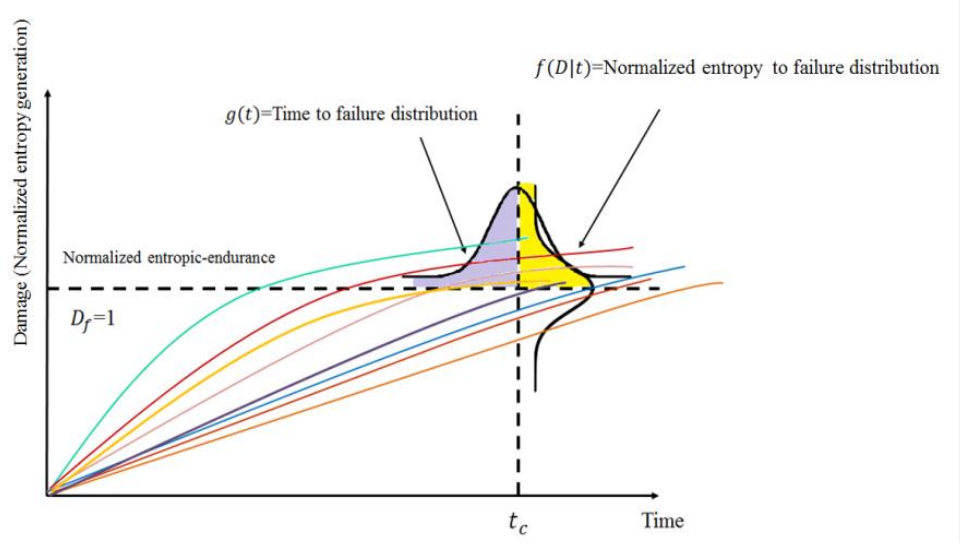
T = temperature, z_M =number of moles of electrons exchanged in the oxidation process, F =Farady number, $J_{M,a}$ and $J_{M,c}$ = irreversible anodic and cathodic activation currents for oxidation reaction, $J_{O,a}$ and $J_{O,c}$ =anodic and cathodic activation currents for reduction reaction, $E_{M_{act,a}}$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

[1] Imanian, A. and Modarres. M, "*A Thermodynamic Entropy Based Approach for Prognosis and Health Management with*

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 [8]

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

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

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

[8] 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).

Entropy Originated from Statistical Mechanics

- Forward / reverse process representing equations in statistical mechanics

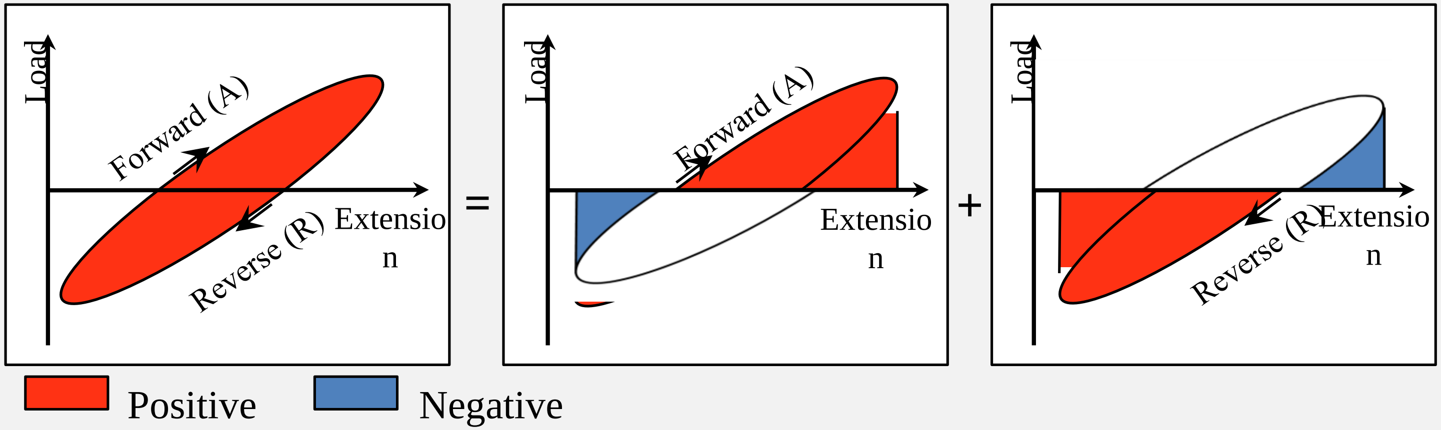
$$\frac{\pi_F\ (+W)}{\pi_R\ (-W)} = exp\left[\frac{W-\Delta F}{k_B T}\right]$$

Crooks' fluctuation theorem

[6]

$$\frac{W_F^{diss}}{k_B T} = \frac{\langle W_F \rangle - \Delta F}{k_B T} = D(\pi_F|\pi_R) = \int \pi_F ln\left(\frac{\pi_F}{\pi_R}\right)$$

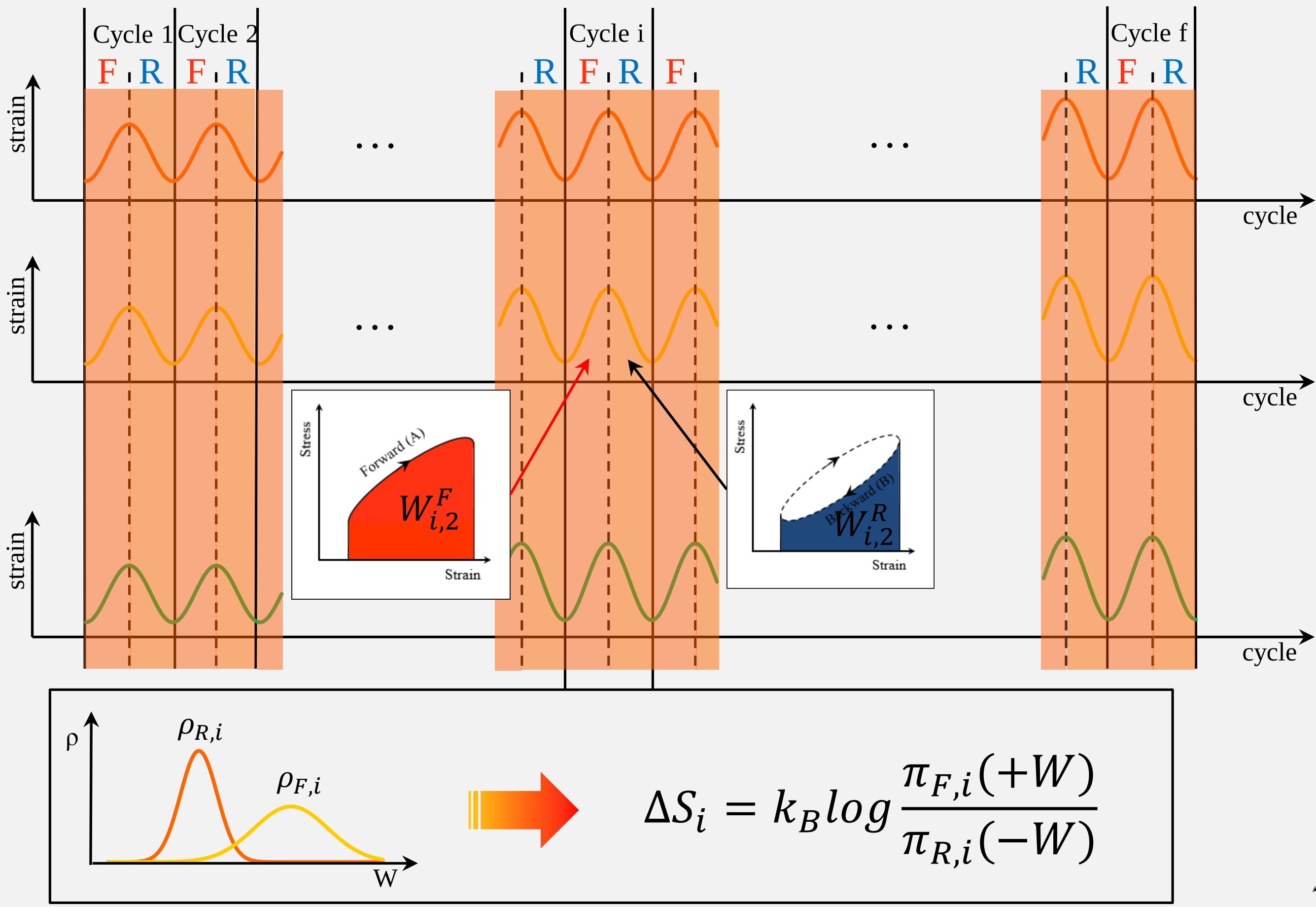
Relative entropy



[6] 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

Statistical Mechanics Entropy

- Schematics of Entropy Computation



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