Entropic methods to study the evolution of damage and degradation of materials

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Acknowledgments

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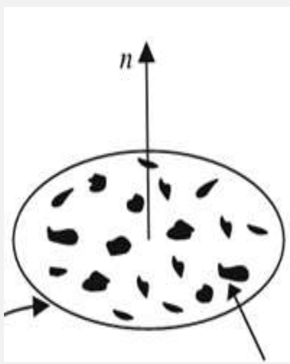
Objectives

- Describe damage resulted from failure mechanisms within the irreversible thermodynamics framework
- Improve understanding of the coupled failure mechanisms
- Define reliability in the context of the 2nd 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

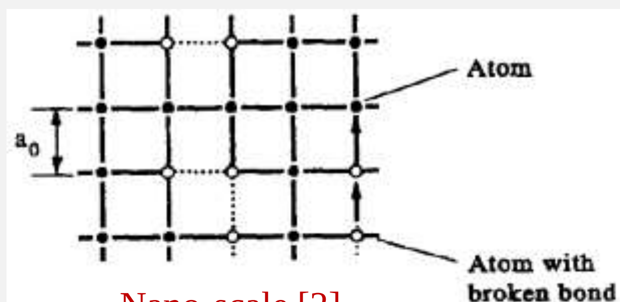
- Common definitions of damage are based on observable markers of damage which vary at different geometries and scales
  - Macroscopic Markers of Damage (e.g. crack size, pit densities, weight loss)
  - Macroscopic Fatigues Markers include: crack length, reduction of modulus, reduction of load carrying 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



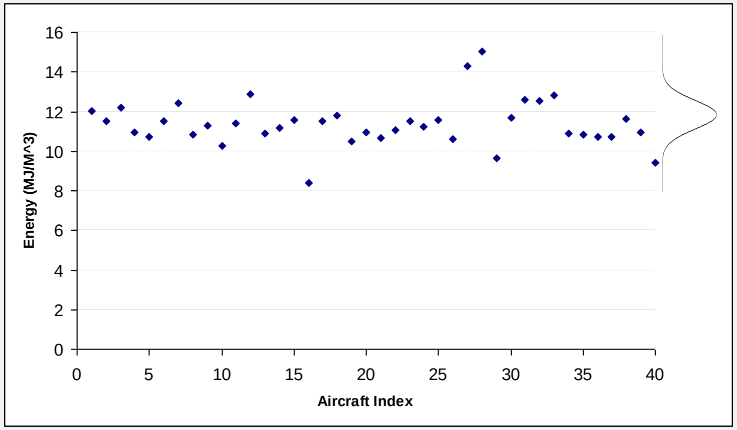
Nano-scale [2]

Meso-scale

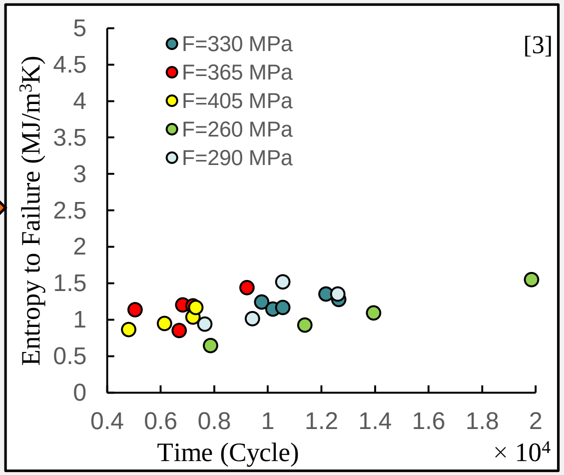
[1] J. Lemaitre, "*A Course on Damage Mechanics*", Springer, France, 1996.
[2] C. Woo & D. Li, "*A Universal Physically Consistent Definition of Material Damage",* Int. J. Solids Structure, V30, 1993

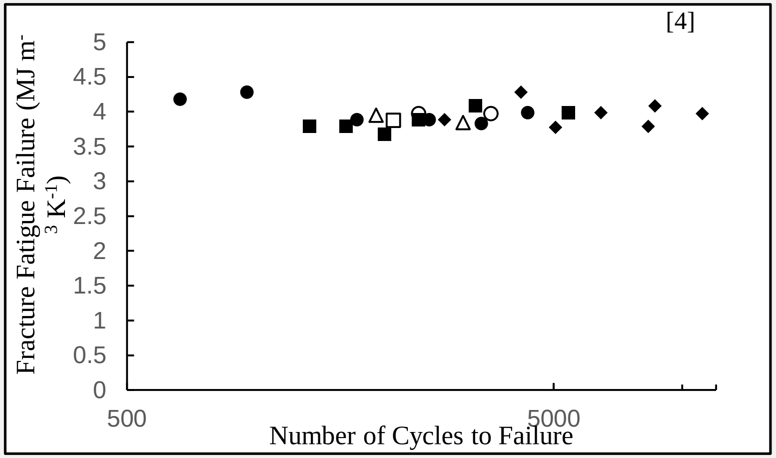
Motivation (Cont.)

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

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**
  - $S = \sum p_i \log p_i$

Approaches to derive and quantify entropy (Cont.)

Entropy

Statistical mechanics

- Repetitive experiments of same conditions to find distribution of work
- Forward and backward work measured

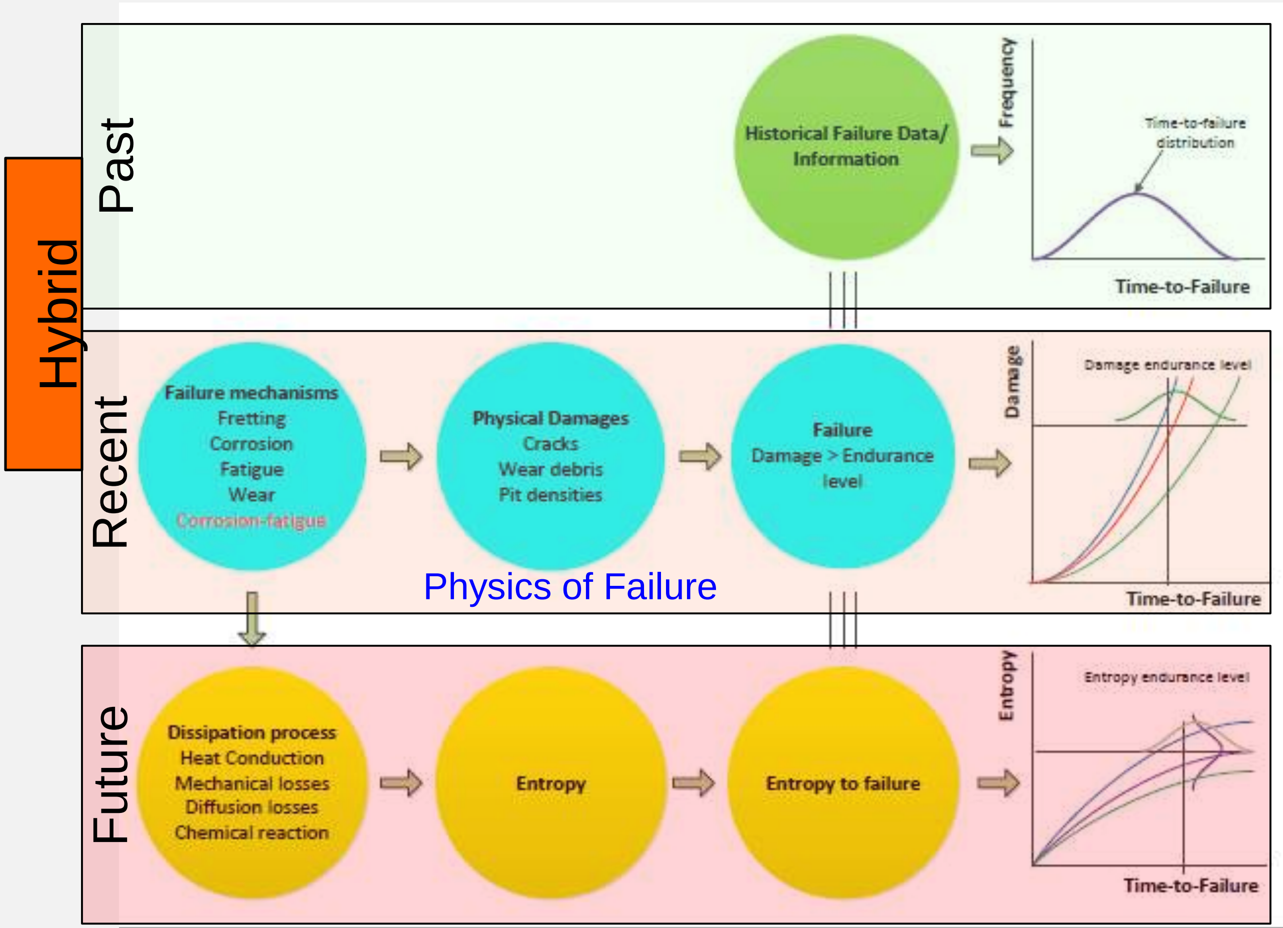
Classical thermodynamics and continuum mechanics

- Entropy generation defined based on thermodynamic forces and fluxes measured

Information theory

- Shannon's entropy of signals as surrogates to damage is calculated

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[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

Total Entropy Generated

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

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

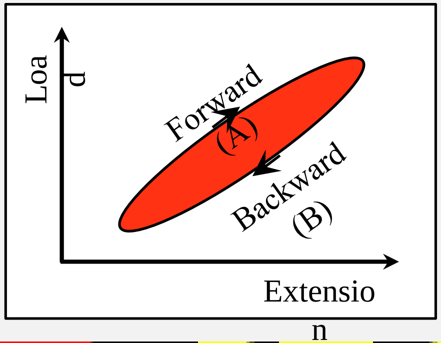
- Entropy generation of important dissipation phenomena leading to damage:

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 *, **



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

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

Entropy Generation in Corrosion-Fatigue

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

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

$$+ \sigma_H$$

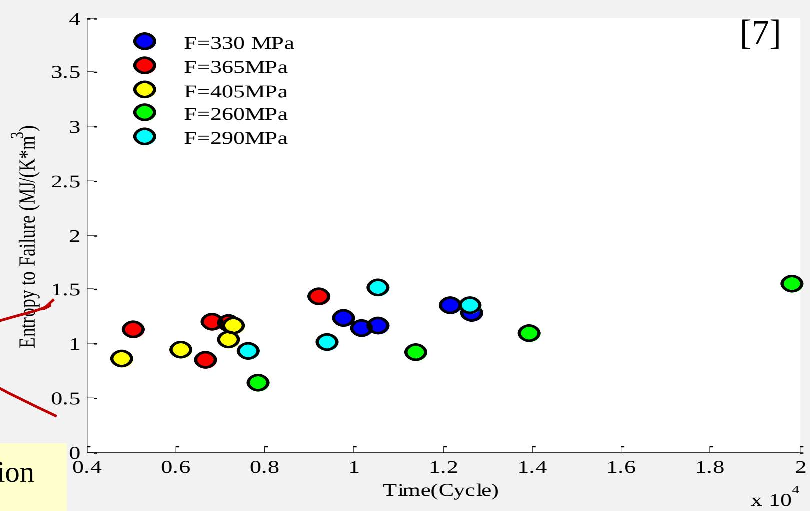
Hydrogen embrittlement dissipation

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.

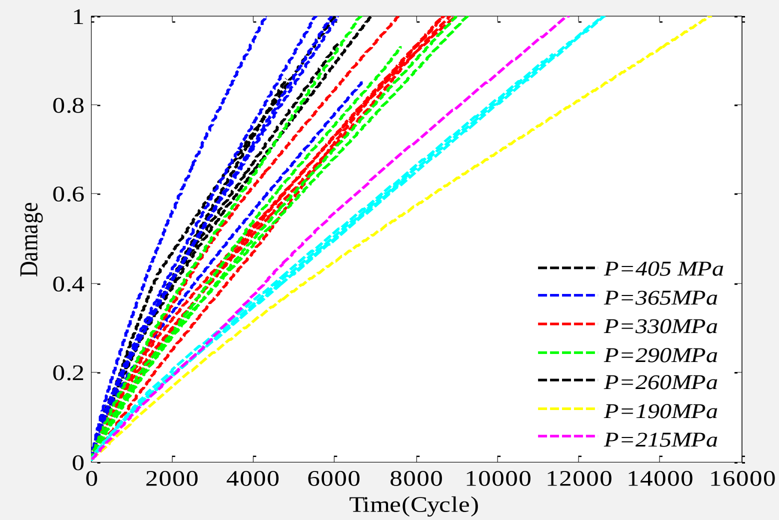
[1] Imanian, A. and Modarres. M, “*A Thermodynamic Entropy Based Approach for Prognosis and Health Management with*

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 future confirm the theory



Distribution of entropic-endurance

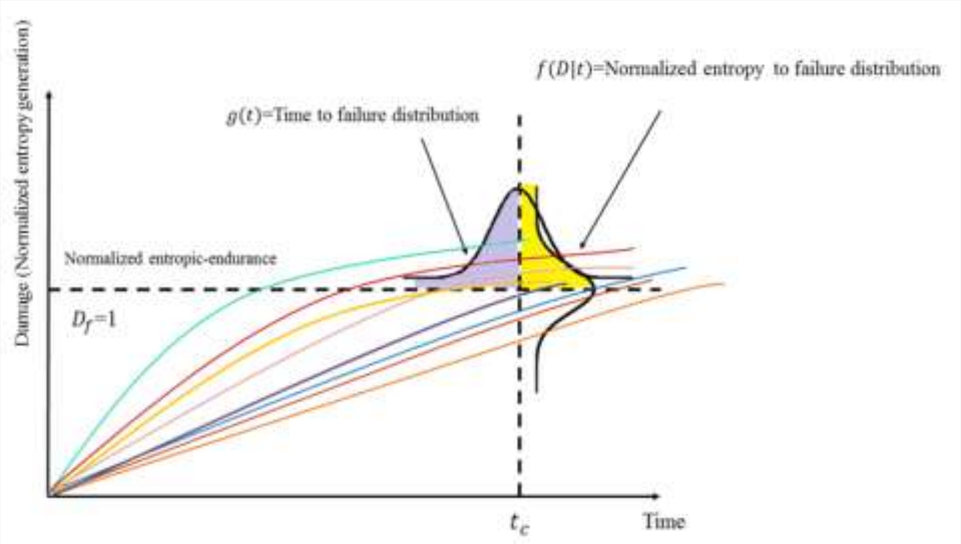


[7] Mohammad Modarres, A General Entropic Framework of Damage: Theory and Applications to Corrosion-Fatigue, Structural Mechanics TIM 2015, 25-26 June 2015, Falls Church, VA, USA

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]

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

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

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).

Statistical Mechanics Entropy

- Theoretical Basis for Acquiring Entropy
  - First law of thermodynamics

Internal energy | Flow of energy into the system | Applied work on the system

$$\Delta U = Q + W$$

by the work protocol

$$U_B - U_A = Q + W$$

  - From Helmholtz free energy

$$F = U - ST$$

$$\Delta F = F_B - F_A = U_B - U_A - (S_B - S_A)T$$

$$\Delta F = \Delta U - T\Delta S$$

$$\Delta F = W + Q - T\Delta S$$

$$\frac{W - \Delta F}{T} = \Delta S - \frac{Q}{T} = \Delta S_{total}$$

$$\frac{\pi_F(+W)}{\pi_R(-W)} = e^{\frac{W-\Delta F}{k_B T}} \quad [5]$$

$$\Delta S_{total} = k_B \log \frac{\pi_F(+W)}{\pi_R(-W)}$$

[5] 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

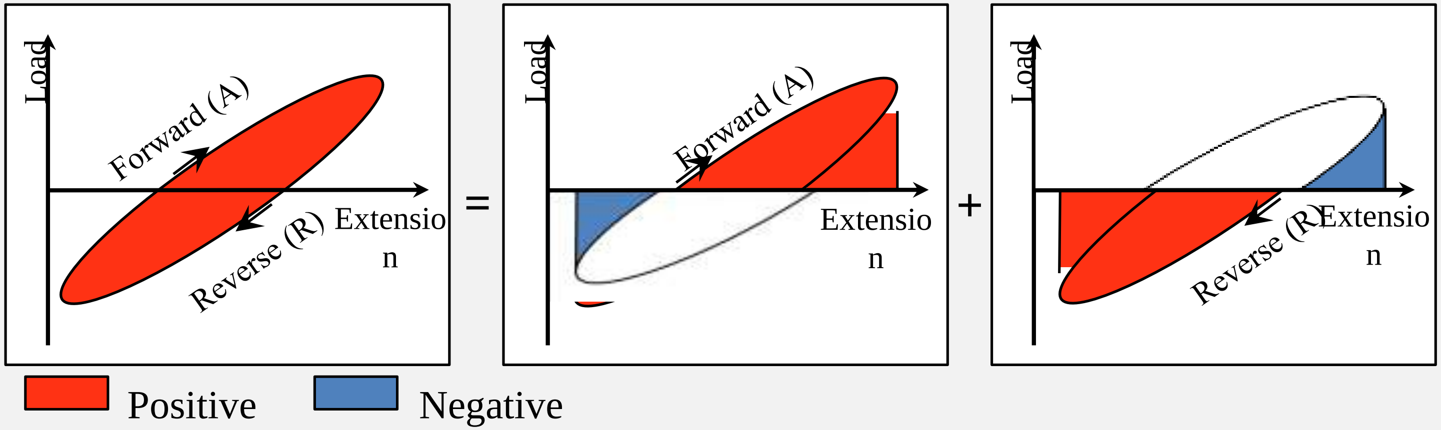
$$\frac{\pi_F\ (+W)}{\pi_R\ (-W)} = exp\left[\frac{W - \Delta F}{k_B T}\right]$$

Crooks' fluctuation theorem

[6]

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

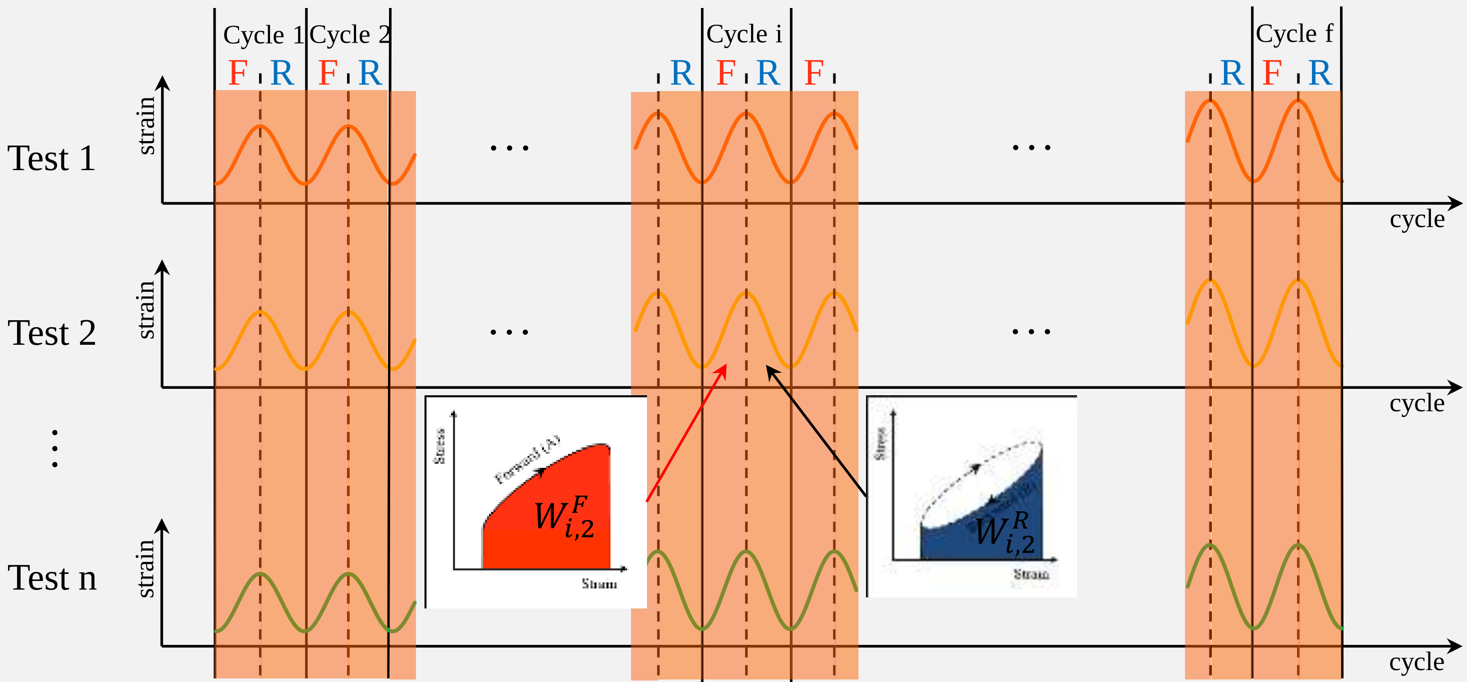
Relative entropy

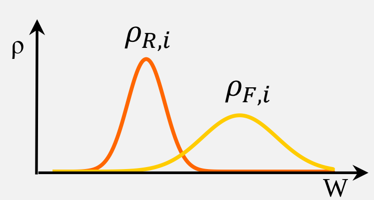


[6] C. Jarzynski, Equalities and Inequalities: Irreversibility and the Second Law of Thermodynamics at the Nanoscale, Annu. Rev. Condens. Matter Phys. 2.1 (2011): 329-351

Statistical Mechanics Entropy

- Schematics of Entropy Computation

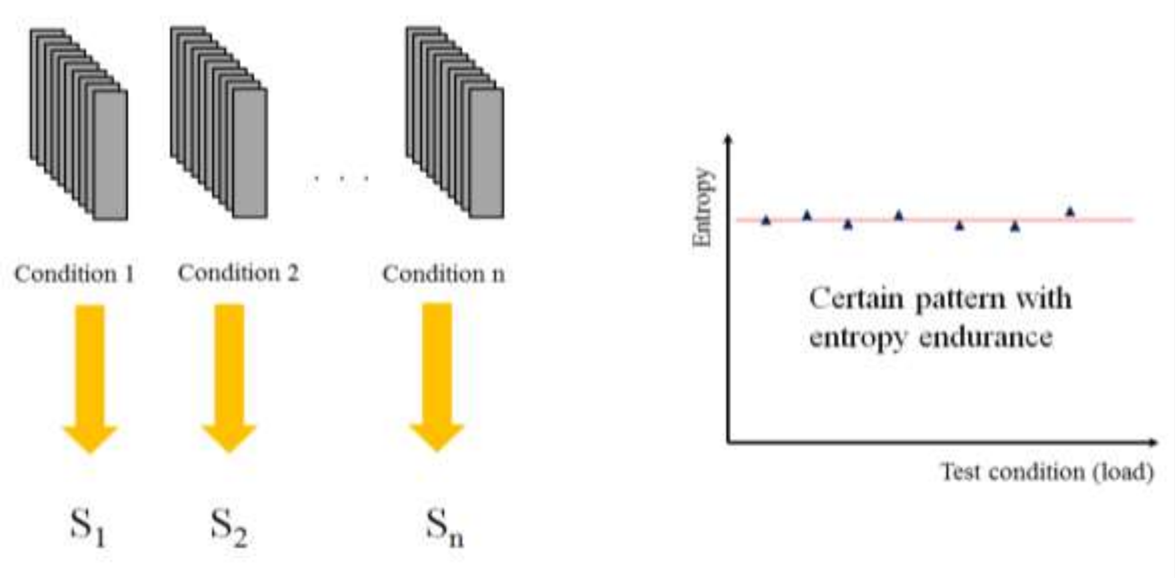




$$\Delta S_i = k_B log \frac{\pi_{F,i}(+W)}{\pi_{R,i}(-W)}$$

Further Verification Needed

- Crook's fluctuation theorem is developed in microscale. The validity of such theorem needs to be investigated in macroscale where the source of fluctuations might be different from microscale.
- More experiments needs to be performed in different experimental conditions to investigate the existence of the entropic endurance limit.
- Benefit: Temperature measurements are not required



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