LIFE PREDICTION WITHOUT CURVE FITTING MODELS:
USING ENTROPY TO UNIFY NEWTONIAN MECHANICS AND THERMODYNAMICS

Prof. Cemal Basaran

Dept. of Civil, Structural and Environmental Engineering
University at Buffalo

Presentation Outline

I- Objective

II- Introduction

III- Historical Efforts to Unify Mechanics and Thermodynamics

IV- Theory

V- Mathematical Verifications

VII- Experimental Verifications

VIII- Conclusions

Objective

Accurately predicting life span of physical bodies - living and non-living – has been humankinds' eternal endeavors.

Newtonian Mechanics versus Thermodynamics

Newtonian Mechanics provides the response of physical bodies to external disturbances, but does not take into account past-present-future changes, like aging, microstructural re-organizations and others.

Thermodynamics, provides information about the past-present-future changes happening in a physical body over time, but does not give any information about the response of a body to any external disturbance.

Newtonian Mechanics

Sir Isaac Newton's work in "The Principia," 1687

First law: an object either remains at rest or continues to move at a constant velocity unless acted upon by a force

Second law: the vector sum of the forces F on an object is equal to the mass m of that object multiplied by the acceleration a of the object: $F = ma$.

Third law: When one body exerts a force on a second body, the second body simultaneously exerts a force equal in magnitude and opposite in direction on the first body.

Historical Efforts

In 1850 Rudolf Clausis and William Thompson (Kelvin) formulated both the First and Second Laws of Thermodynamics

between 1872 and 1875 , Using statistical mechanics, Boltzmann's formulated probability equation relating the entropy to the quantity disorder.

1934, Swiss physical chemist Werner Kuhn successfully derived a thermal equation of state for **rubber** molecules using Boltzmann's formula. **[Boltzmann's formulation is not restricted to gasses, as Boltzmann indicates]**

Historical Efforts to Introduce Thermodynamics into Mechanics

Since Newtonian mechanics does not account for past, present and future. There were many attempts to introduce degradation into mechanics, such as:

- Stress-Number of Cycles (S-N) curve
- Miner's Rule
- Coffin-Manson
- Paris' Law
- Gurson Model
- Gurson-Tvergaard-Needleman Model
- Johson-Cook Model
- Structural Fragility Curves
- “Kachanov” Damage Mechanics Models- damage potential surface

Problem with Historical Efforts

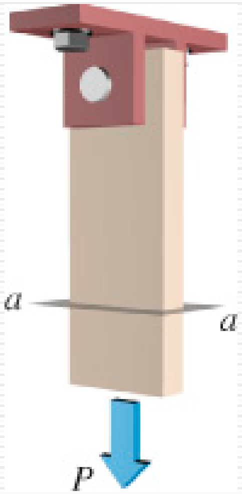
- They are all based on phenomenological curve fitting techniques. Degradation response is needed before-hand to generate a polynomial.
- Most do not satisfy laws of thermodynamics, due to using displacement, strain or stress.
- They are only valid for the test tyoe and specimen size they are obtained for.
- They require linear superposition of many damage mechanisms due to different load types (Miner's rule)
- Results cannot be extrapolated to any other loading path or outside their range.
- Most cannot account for past.

Unified Theory –
MechanoThermodynamics

Both displacement (or force), entropy generation rate are nodal unknowns.

Newtonian Mechanics u= P/k

u doesn't change by time



MechanoThermodynamics

New Nodal unknowns

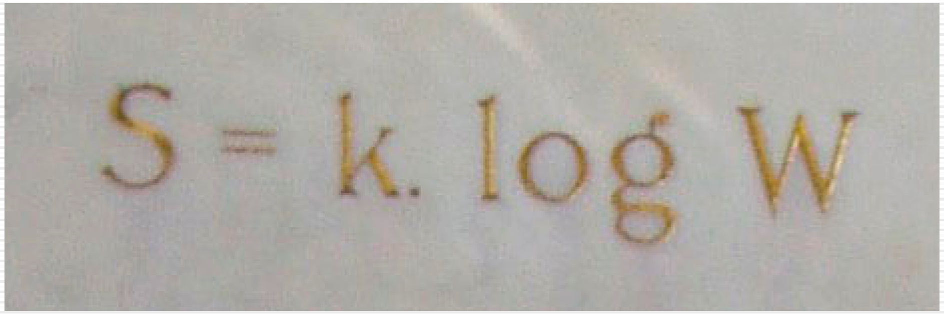
u, $\dot{\gamma}$

NO CURVE FITTING, or PHENOMENOLOGICAL MODELs

2nd Law of Thermodynamics

The Second Law states that there is a natural tendency of any isolated system, living or non-living, to degenerate into a more disordered state.

When **irreversible entropy generation** becomes zero the system reaches “THE END” (fails/dies).



Boltzmann's equation—carved on his gravestone.

The logarithmic connection between entropy and disorder probability was first stated by L. Boltzmann (1872) and put into final form by Maxwell Planck (1900)

<u>Note that Boltzmann formulates this hypothesis for an arbitrary body, i.e. formulation in the original paper is NOT restricted to gases.</u>

Everything in Nature , [living and non-living] is a Thermodynamic System

Entropy (S) of a system can be related to probability (W) of existence of the system to be at a microstructural (disorder) state with respect to all other possible microstructural (disorder) states.

Thermodynamic State Index (TSI):D

Let that probability of a material being in a completely ordered ground state is equal to W_o

under external loads (mechanical, thermal, electrical, chemical, radiation, corrosion and environmental), material deviates from this reference state to another disordered state with a probability of W.

$$W_o \dashrightarrow W$$

Irreversible Degradation in Solids

External effects will lead to permanent changes in microstructure of the material described as a positive entropy production. In solids "damage" happens due to ***irreversible internal entropy production.***

Since a disordered state is formed from an ordered state due to "damage" (TSI change), "damage" and entropy (which is a measure of disorder) are related.

Reference Thermodynamic States

When a material in ground (reference) state, it is free of any possible defects, i.e. damage, it can be assumed that "damage" in material is equal to zero. TSI will be D= 0.

In final stage, material reaches a critical state such that disorder is maximum, W_{max}. At this stage, entropy production rate will become zero. TSI will be maximum D = 1.

Thermodynamic State Index

In order to relate entropy and damage, consider a system in ground state D= 0 with a total entropy of S_o and an associated disorder probability is Wo

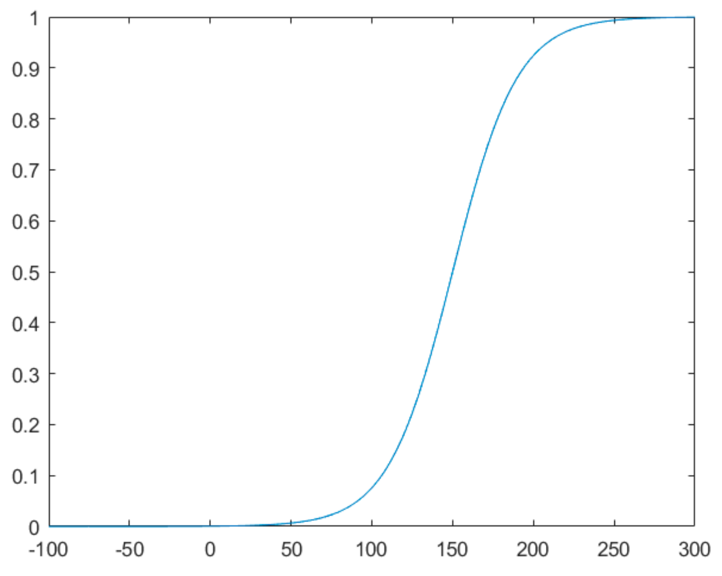
In an alternative disordered (damaged) state, S is total entropy of the same system with an associated probability of W and a TSI level of D.

Instantaneous value of TSI can be calculated by the difference in TSI probability from the ground state probability $D = f(W - W_o)$

Universal Damage Evolution

TSI value must be normalized w.r.t. disorder probability in current state. Therefore;

$$D = f\left[\frac{W - W_o}{W}\right]$$



Multi Physics Entropy Computation

$$\Delta s = \int_{t_o}^{t} \frac{1}{\rho} \dot{\gamma} \, \mathrm{dt}$$

$$\Delta s = \int_{t_0}^{t} \left\{ \begin{array}{l} \frac{1}{\rho T^2} k_T \left| Grad(T) \right|^2 + \frac{r}{T} \\ \frac{C_v D_{effective}}{\rho k_B T^2} \left[Z_l^* e \rho^* j - f \Omega \nabla \sigma_{spherical} + \frac{Q^* \vec{\nabla} T}{T} + \frac{k_B T}{c} \vec{\nabla} C \right]^2 \\ + \frac{1}{\rho T} \boldsymbol{\sigma} : \boldsymbol{\varepsilon} \end{array} \right\} dt$$

Irreversible Entropy Production due to

1- Internal heat generation

2- Diffusion mechanisms (Electromigration, stress gradient, thermomigration, and vacancy (chemical) concentration gradient

3- Internal mechanical work

Entropy Computation does not Require any Curve Fitting Parameters

Where C_v vacancy concentration, $D_{effective}$ vacancy diffusivity

Z^* is vacancy effective charge number

e is electron charge

ρ^* is metal resistivity

$\mathbf{j}$ is current density (vector)

f is vacancy relaxation ratio

Ω is atomic volume

k is Boltzman's constant

T is absolute temperature

C is normalized vacamcy comcentration $c=C_V/C_{VO}$

C_{vo} equilibrium vacancy concentration

in the absence of stress field

$\sigma_{spherical}$ is spherical part of stress tensor,

$$\sigma_{spherical} = trace(\sigma_{ij})/3$$

Q^* is heat of transport

Mathematical Proof

Provided in

Leonid A. Sosnovskiy and Sergei S. Sherbakov, **"Mechanothermodynamic Entropy and Analysis of Damage State of Complex Systems"**, ***Entropy*** (2016), 18, 268;

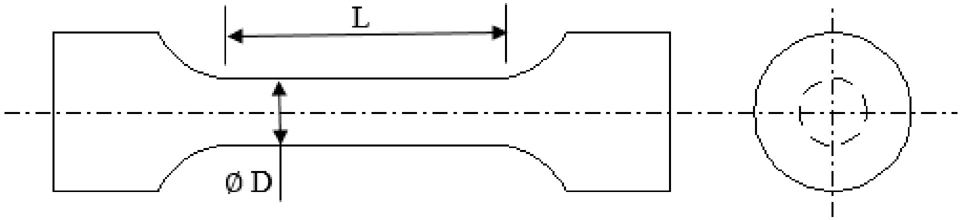
Based on the Concept first published By

Basaran and Yan, ASME J. of Electronic Packaging 120, 379, 384, (1998)

Basaran, C. and Nie, S., **"An Irreversible Thermodynamics Theory for Damage Mechanics of Solids"** *International Journal of Damage Mechanics*, Vol. 13—July 2004

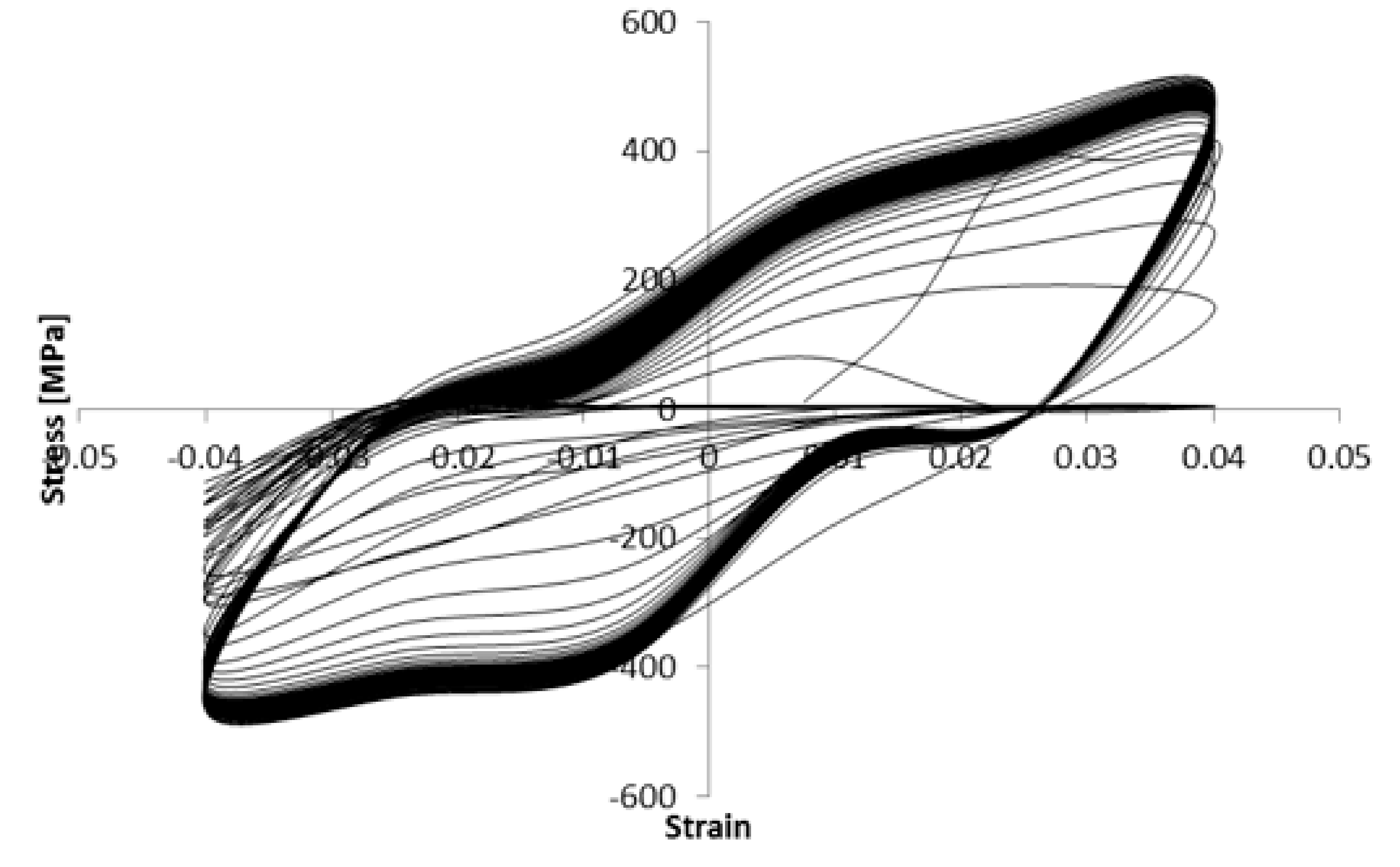
Experimental Verifications

Fatigue Loading on A-36 Steel



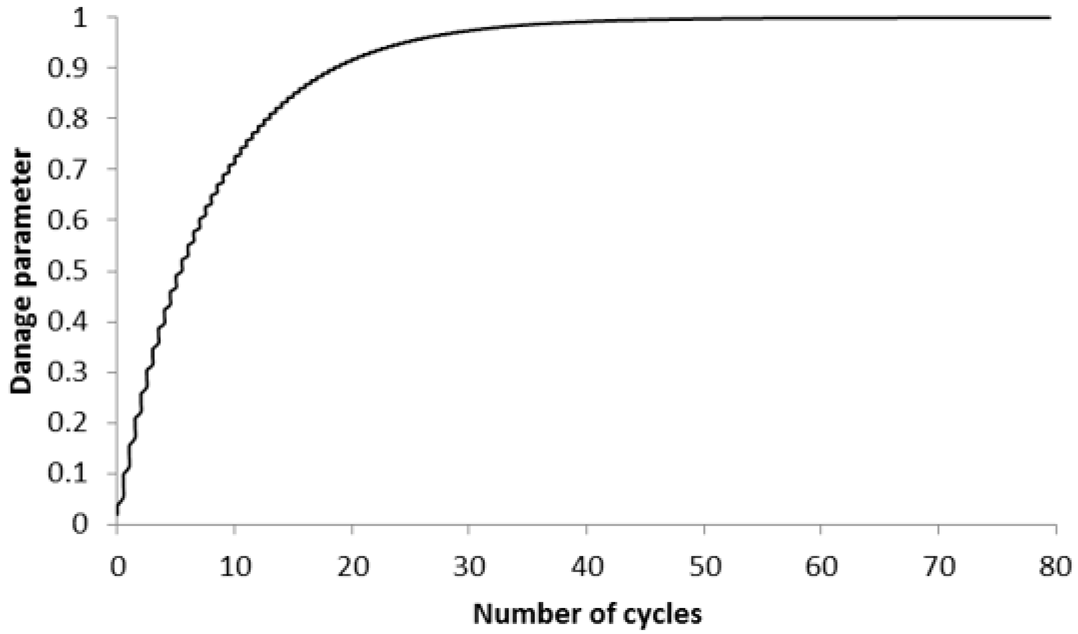
L=25mm	D=6.4mm
E=210000MPa	ν=0.3
T=295K	R=8.314J/K.mol
ρ=7750kg/m^3	m_s=55.8 g/mol

Fatigue Loading – Displacement Controlled Test

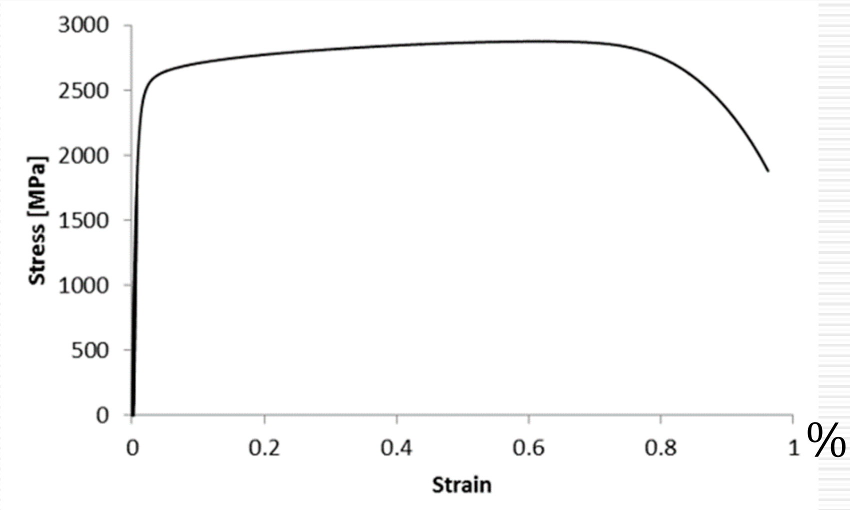


Damage Evolution - Calculated

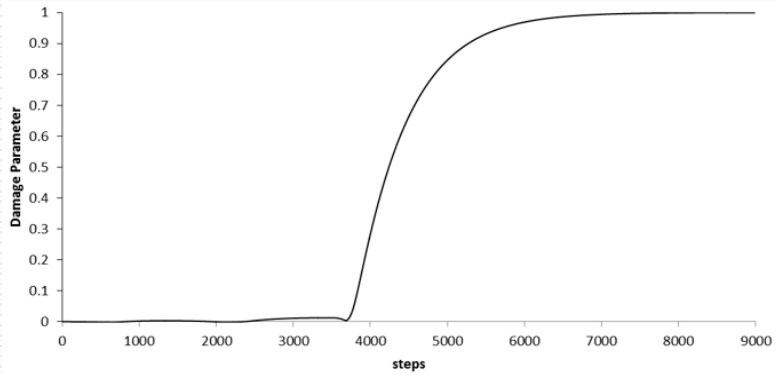
$$\Delta\eta = \int_{t_0}^{t} \frac{\sigma:\dot{\varepsilon}^p}{\rho T} dt$$



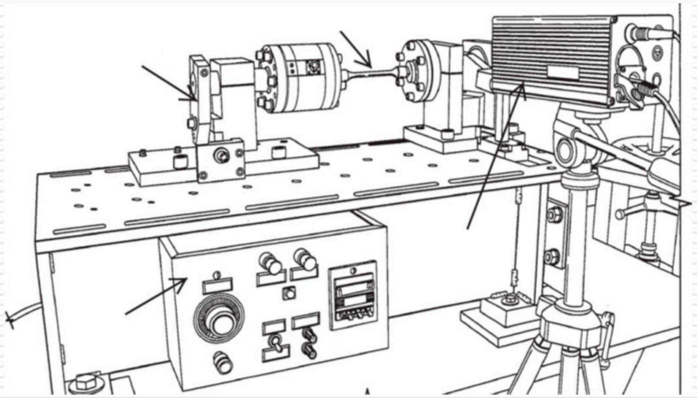
Monotonic Loading Test



Damage Parameter (Thermodynamic State Index)



M. Naderi, M. Amiri and M. M. Khonsari , On the thermodynamic entropy of fatigue fracture" **Proceedings of the Royal Society A** (2010) 466, 423–438



'A thermodynamic approach for the characterization of material degradation, which uses the entropy generated during the entire life of the specimens undergoing fatigue tests is used. Results show that the cumulative entropy generation is constant at the time of failure and is independent of geometry, load and frequency."

Imanian, A., Modarres, M., "A Thermodynamic Entropy-Based Damage Assessment with Applications to Prognosis and Health Management", ***Structural Health Monitoring***, (2017) DOI: 10.1177/1475921716689561

"We therefore conclude that entropy generation can be used to assess the degree of damage, the amount of the life of materials expended and the extent of the life remaining".

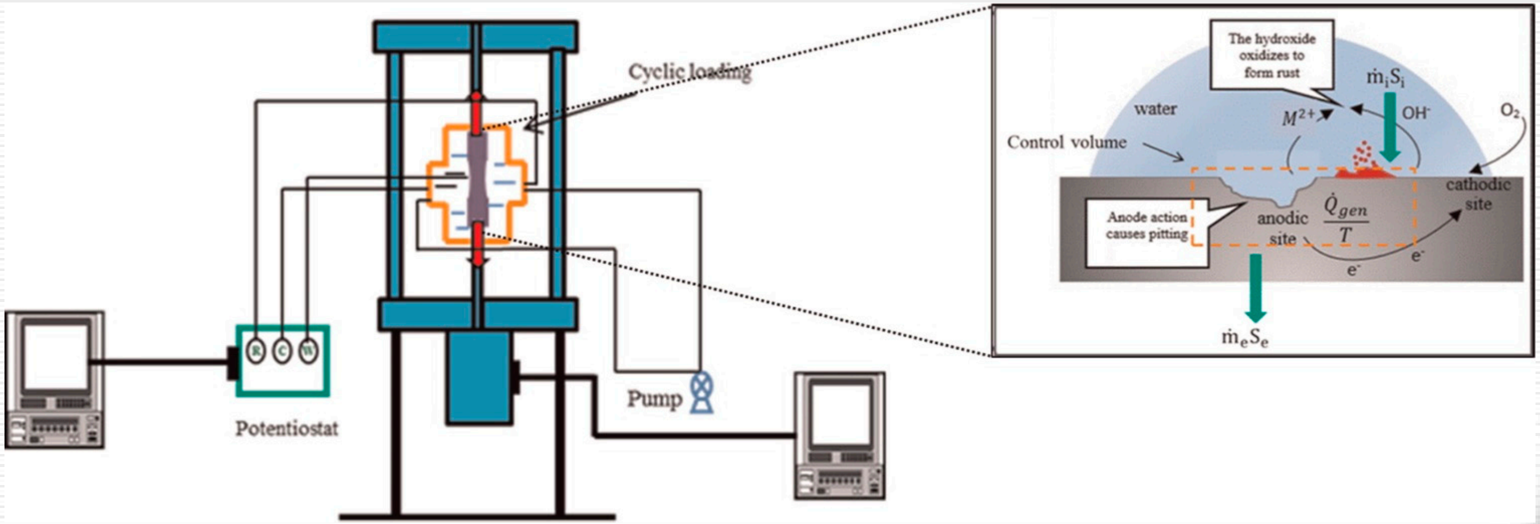
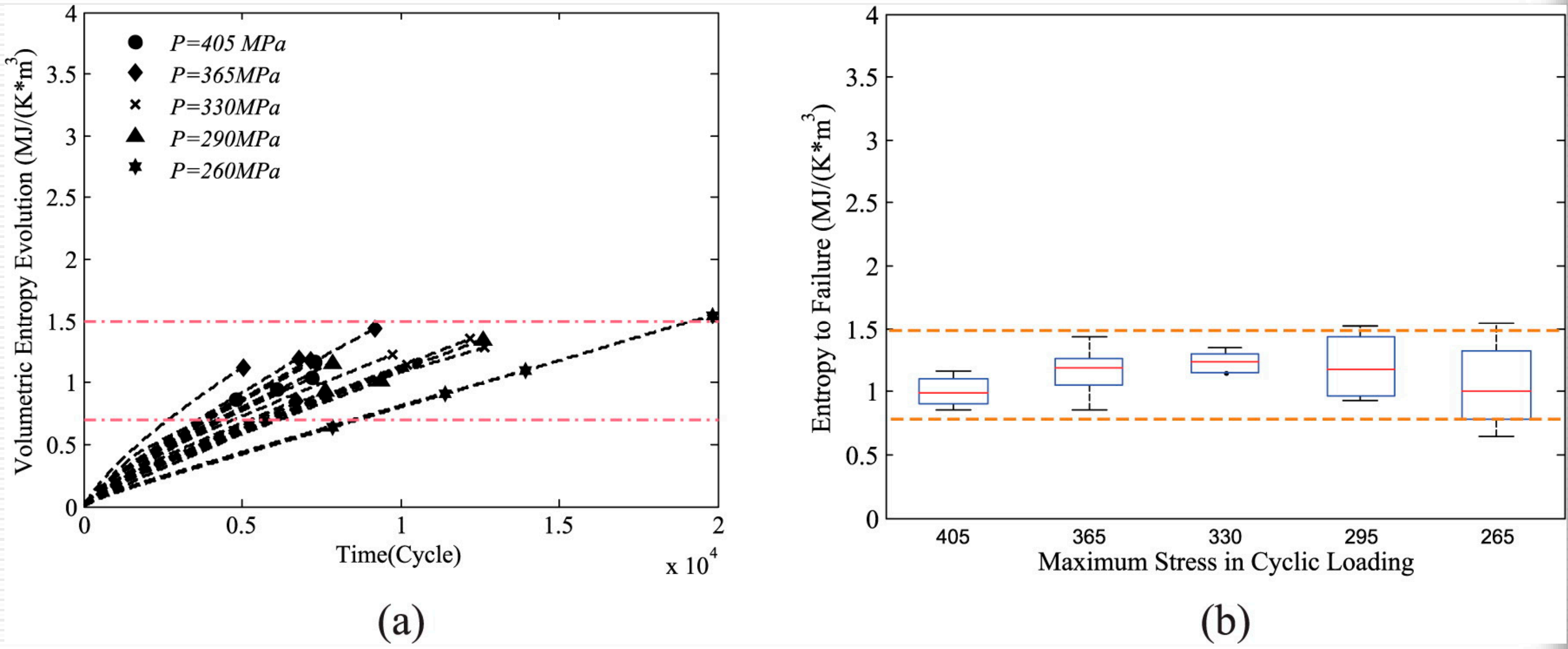


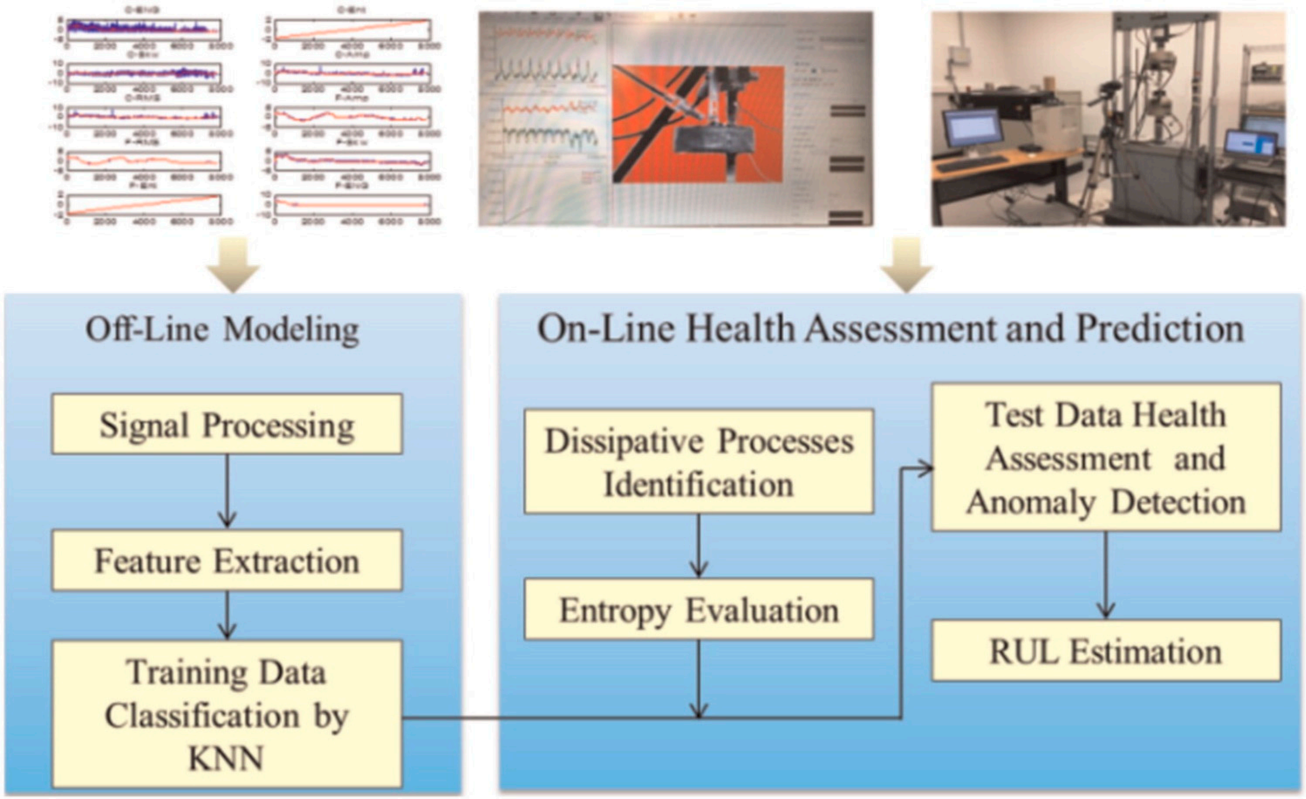
Figure Entropy flow in the control volume under corrosion-fatigue

Electronic Packaging Laboratory
University at Buffalo The State University of New York



Volumetric entropy generation evolution. In the Figure 2(a), *P* represents the tensile stress.

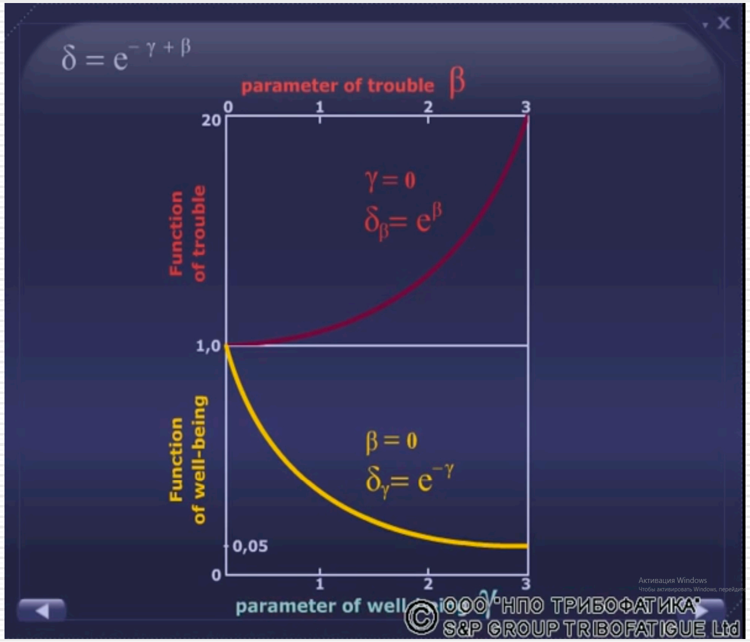
Imanian, A., Modarres, M., “A Thermodynamic Entropy-Based Damage Assessment with Applications to Prognosis and Health Management”, **Structural Health Monitoring**, (2017)
DOI: 10.1177/1475921716689561

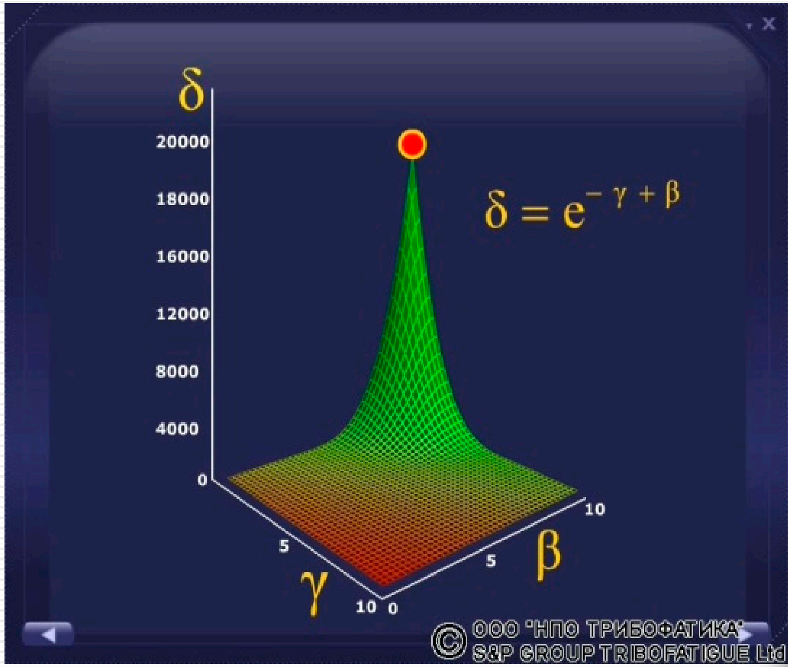


The application of the entropy-based Prognosis Structural Health Monitoring

Leonid A. Sosnovskiy and Sergei S. Sherbakov, "Mechanothermodynamic Entropy and Analysis of Damage State of Complex Systems", Entropy 2016, 18, 268;

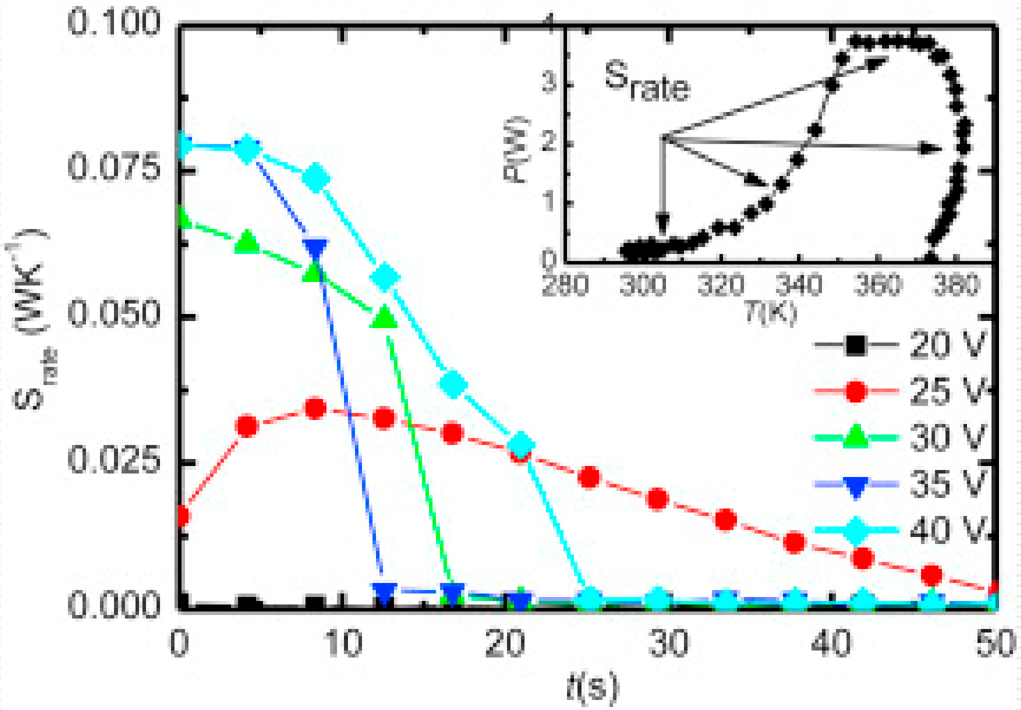
Healing versus Damage





"Life is a special way of existence of [protein] systems that evolve by the inevitable states of irreversible damage"

Angel Cuadras*, Ramon Romero, Victoria J. OvejasEntropy characterization of overstressed capacitors for lifetime prediction, ***Journal of Power Sources***, Volume 336, 30 December 2016, Pages 272–278



"We proposed a method to estimate ageing in electrolyte capacitors based on a measurement of entropy generation rate, S_.."

Time evolution of, entropy generation rate S_ and capacitance for the capacitor 33 mF capacitor biased with a 4 V pulsed excitation.

Angel Cuadras, Jiaqiang Yao, and Marcos Quilez,” Determinationof LEDs degradation with entropy generationrate” **Journal of Applied Physics 2018** (in print)

Conclusions

A correlation between LED’s optical fade and entropy generation rate was found.

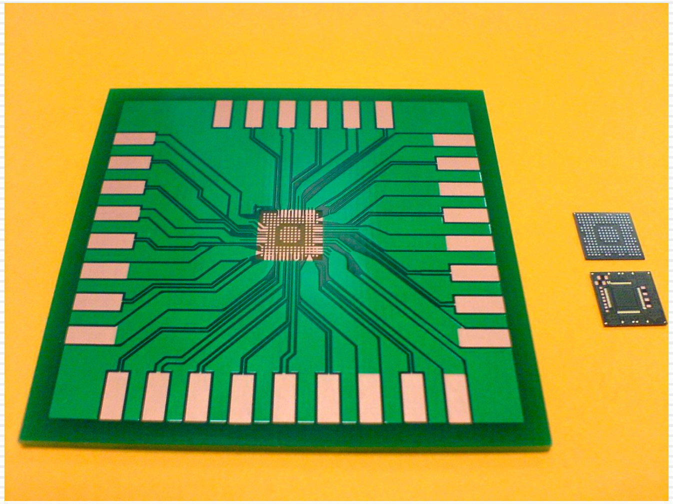
Note: A Light-Emitting Diode is a two-lead semiconductor light source.
It is a p-n junction diode that emits light when activated.

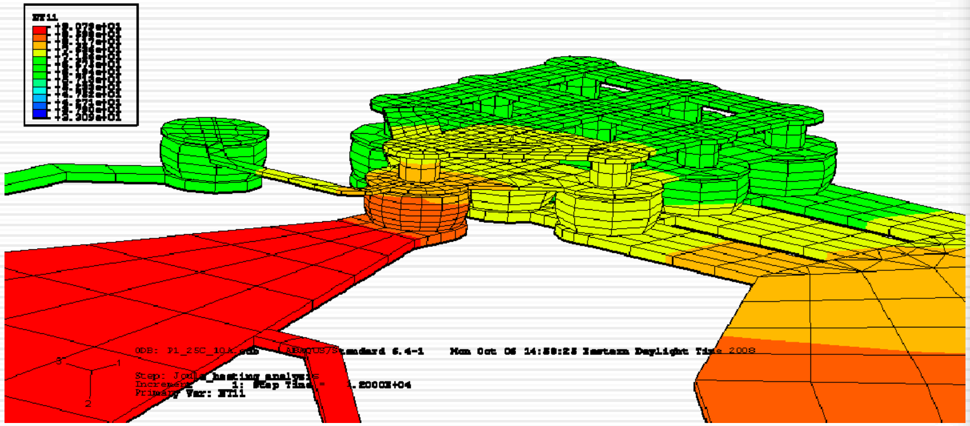
Applications is Dynamical Systems

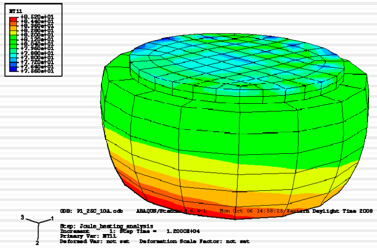
Haddad,W.M. ***A Dynamical Systems Theory of Thermodynamics***; Princeton University Press: Princeton, NJ,2018.

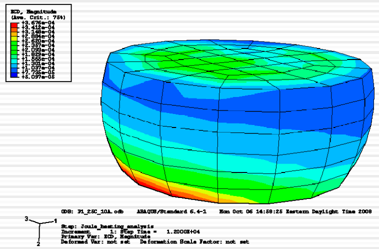
"……. harmonize thermodynamics with classical mechanics [using entropy].

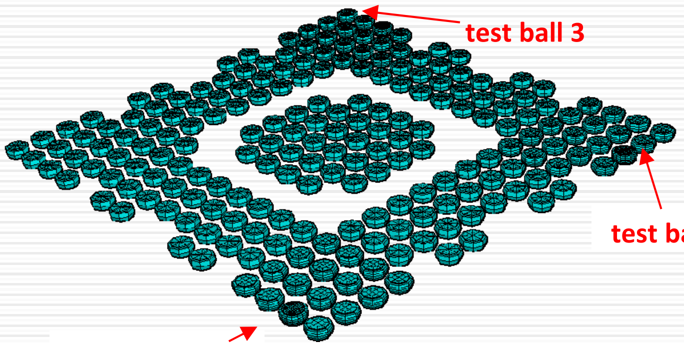
Thermal Cycling of a Computer Chip

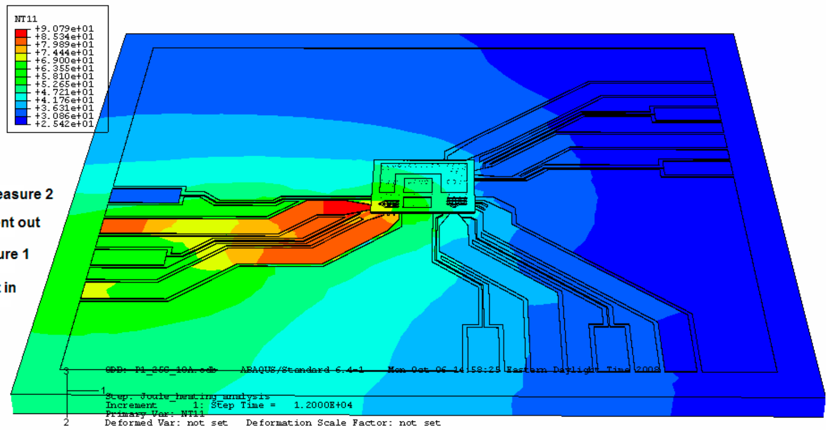




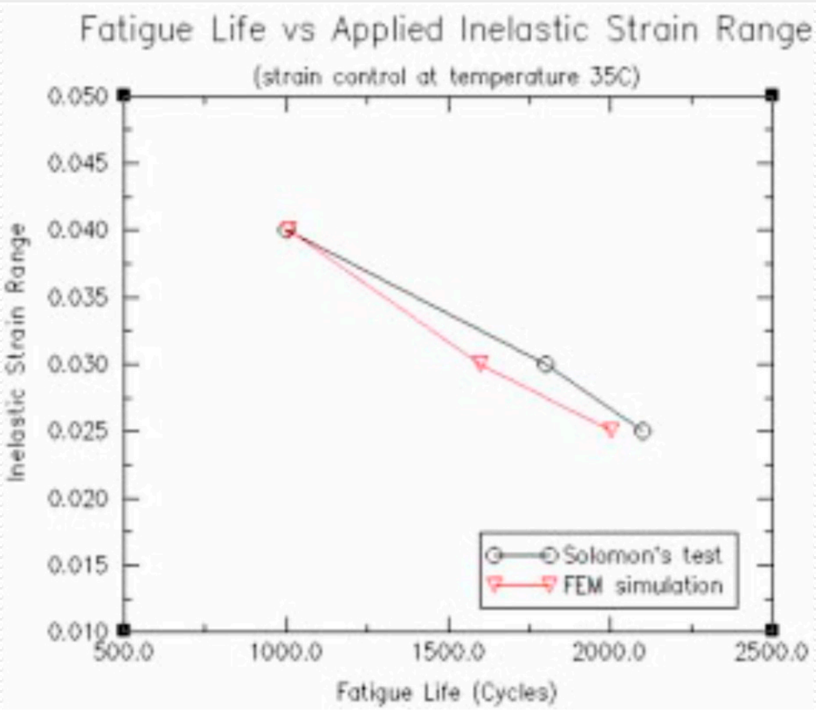


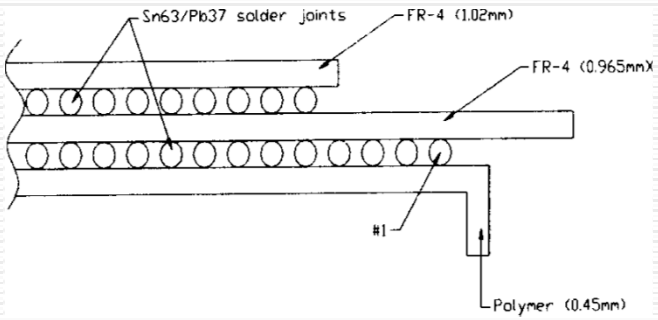


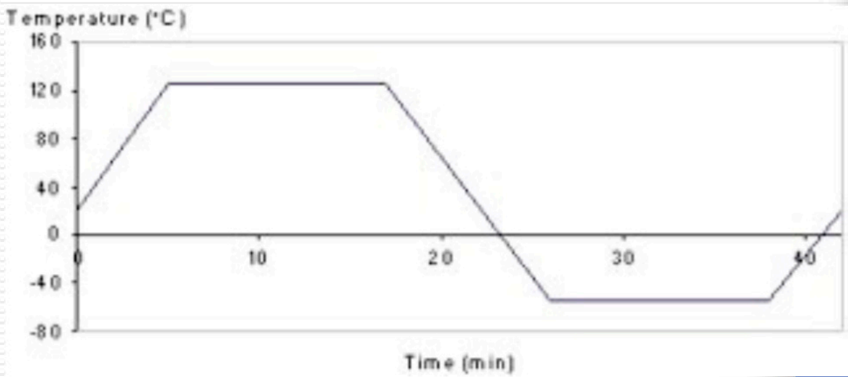




Fatigue due to Temperature Cycling

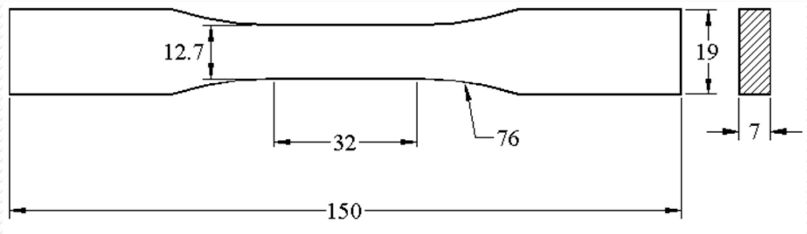


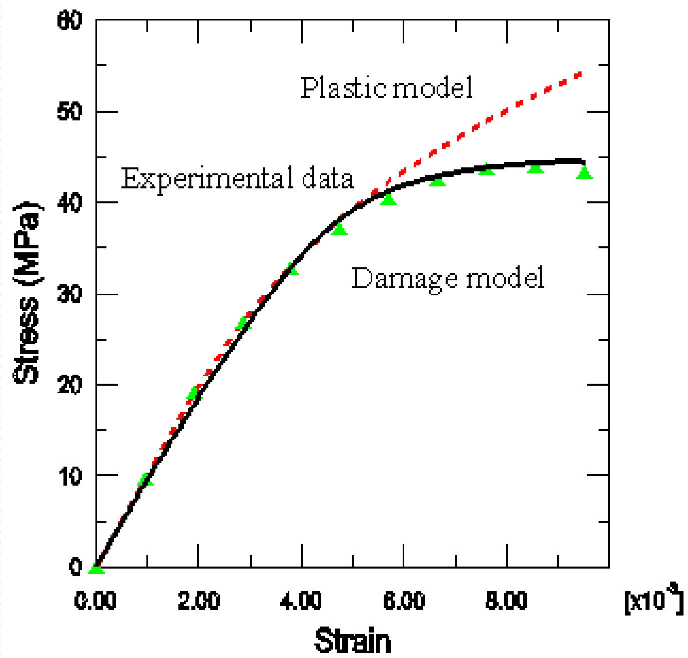


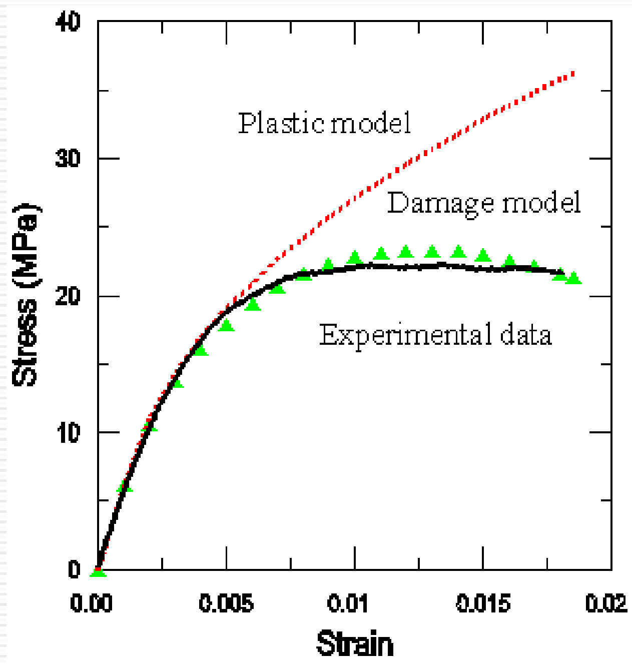


"Implementation of a Thermodynamic Framework for Damage Mechanics of Solder Interconnects in Microelectronic Packaging," **International Journal of Damage Mechanics**, Vol. 11, No. 1, pp. 87-108, January 2002.

Uniaxial tensile test on Particle Filled Composite

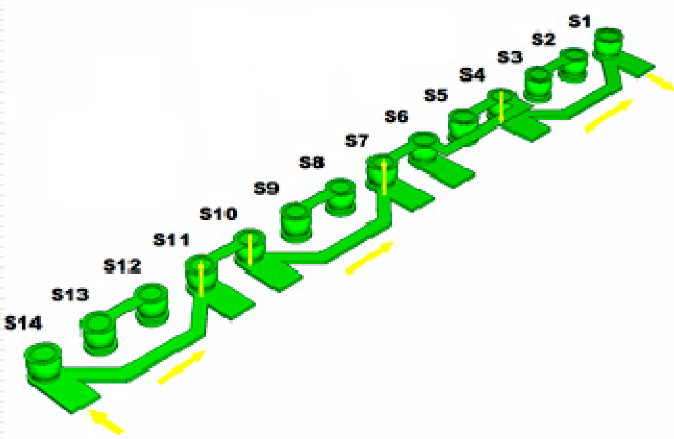


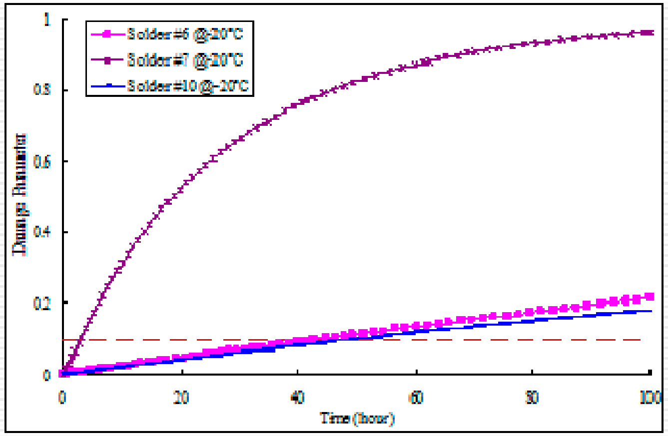




Damage coupled plastic model, Ramberg-Osgood plasticity model and experiment data at 24 ^{0}C and 75^0 C

DAMAGE Due to Combined ELECTROMIGRATION AND THERMOMIGRATION



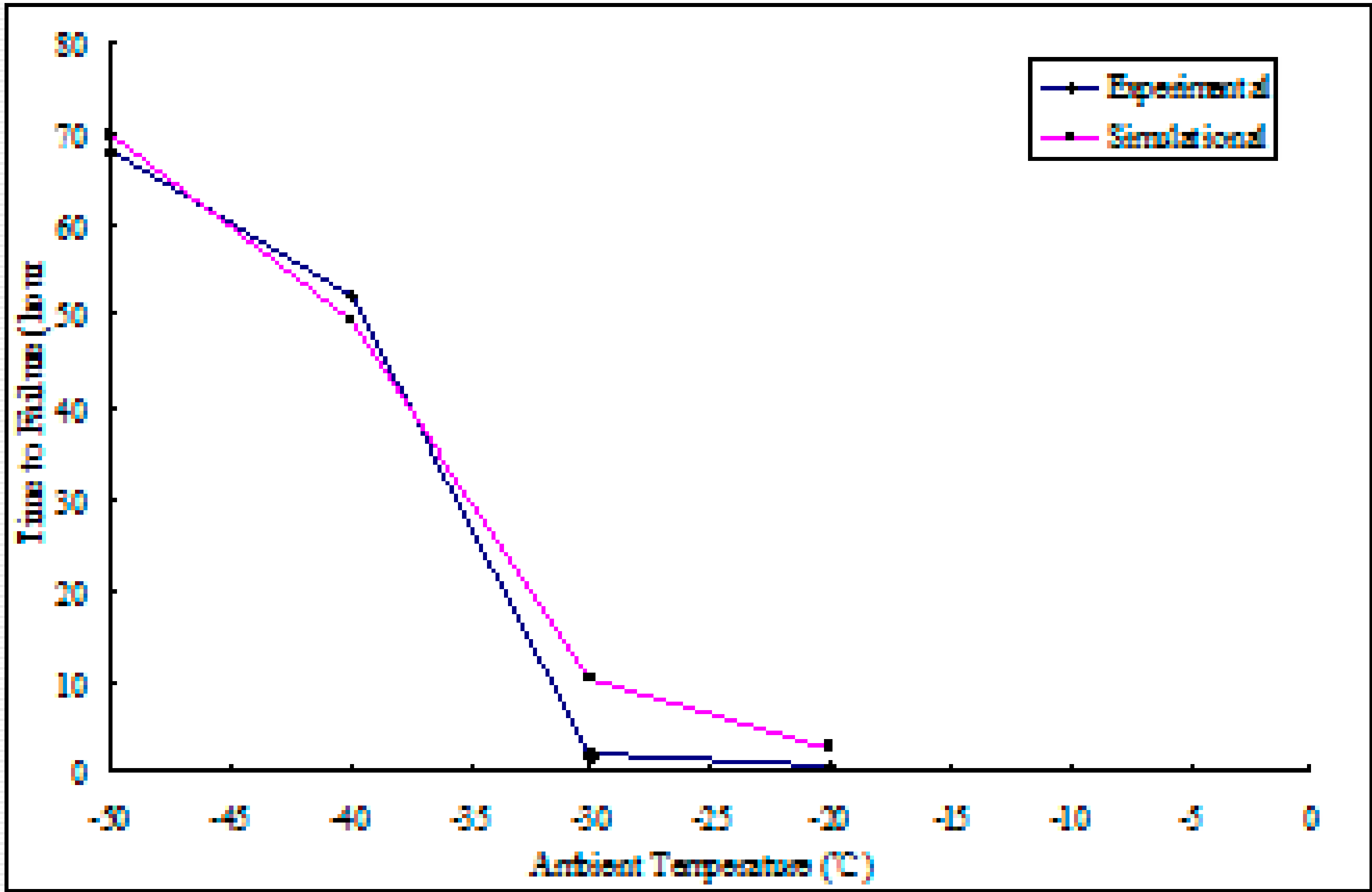


Electrified daisy chain and direction of current

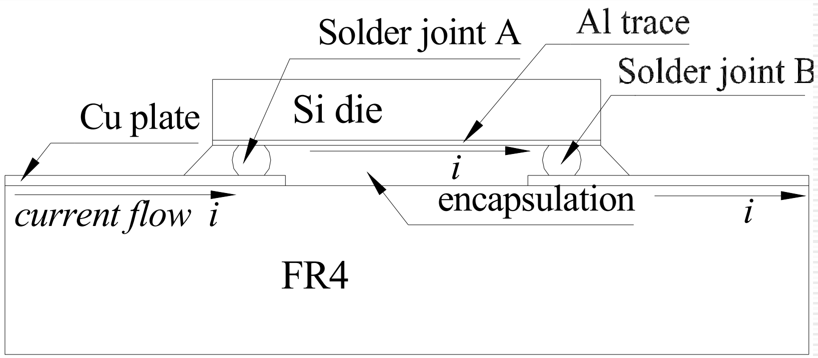
Damage Evolution of 3 solders at -20°C

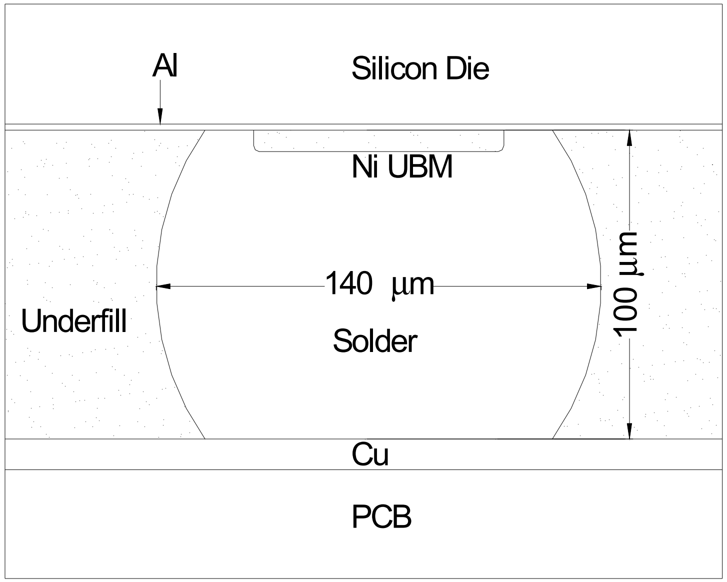
Comparison of Experiment vs Simulation Results

Time to Failure under EM + TM for different Ambient Temp



Damage due to EM + TM

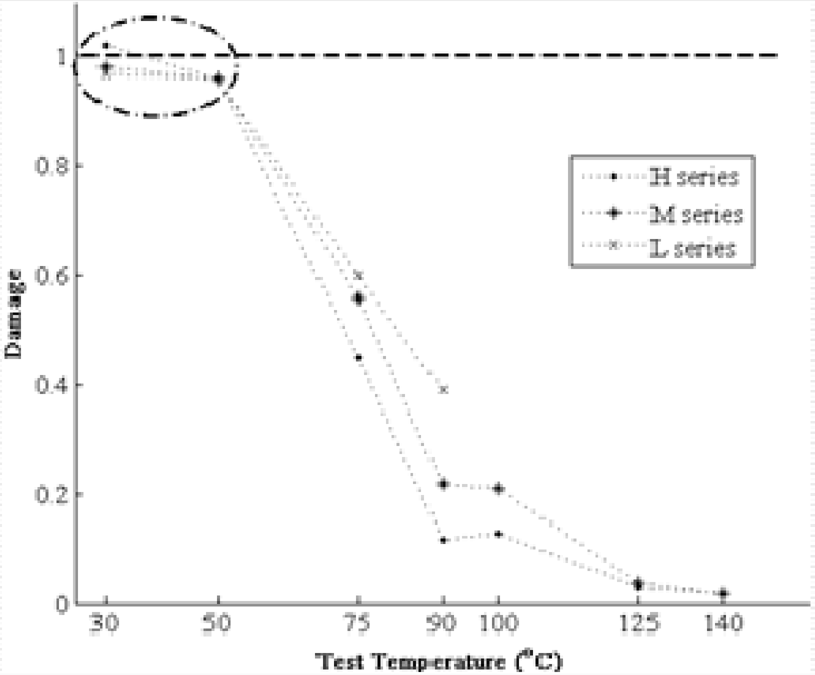


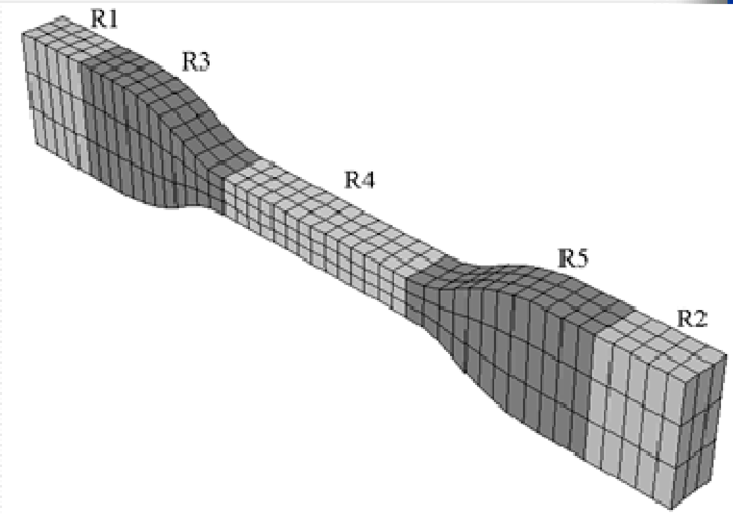


Time to Failure : Simulation vs. Test Data

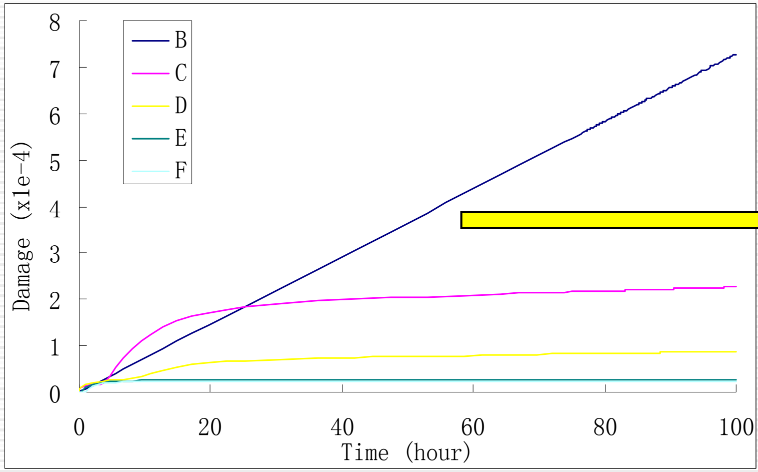
Current Density	Experiment Data TTF=a/j^{3}e $^{(b/T)}$	Simulation Results (D_{cr}=1)
1.0x 10^4 Amp/cm^2	228.7	222.41
0.8 x 10^4 Amp/cm^2	446.6	435.33
0.6 x 10^4 Amp/cm^2	1058.7	1098.2

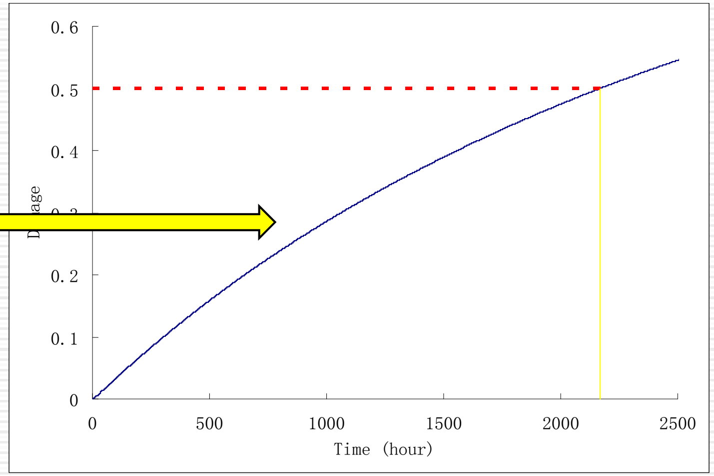
Simulating Polymer Processing

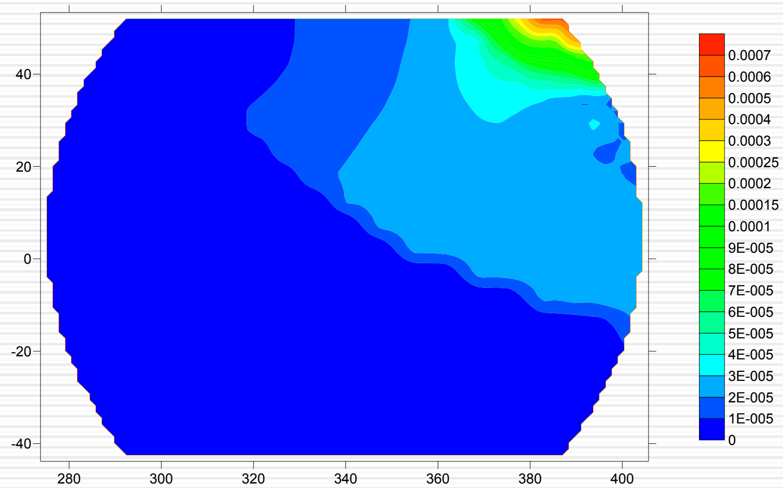




Damage Evolution Distribution during TM







- ➢damage cease to increase after some time in regions (C, D, E, F)
- ➢**When the temperature gradient exceeds a threshold, damage will keep accumulating until it fails.**

CONCLUSIONS

- After 150 years of trying a physics based universal degradation evolution model is possible.

- Entropy based model can predict degradation of Inorganic and "organics" systems under any loading including
  - Mechanical
  - Thermal
  - Chemical
  - Electrical
  - Radiation
  - Corrosion
  - Others

QUESTIONS