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UNIFIED MECHANICS THEORY

Unification of Newtonian Mechanics & Thermodynamics

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Fracture and Lifetime of Materials - In Honor of Prof. Alexander Chudnovsky's 80^{th} Birthday

- **Presentation Outline**
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- I- Objective
- II- Introduction
- III- Literature
- IV- Theory & Mathematical Verifications
- V- Experimental Verifications
- VI- Conclusions

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Objective

- Accurately predicting response of solids without empirical degradation, fracture & fatigue life, curve fitting models.

Newtonian Mechanics vs. Thermodynamics

- **Newtonian Mechanics** provides the response of a structure to external load, but it does not take into account past-present-future changes, i.e. degradation.

- **Thermodynamics**, provides information about the **past-present-future** changes happening in a structure over time.

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Historical Efforts to Introduce Thermodynamics into Newtonian Mechanics

- Stress-Number of Cycles (S-N) curve
- Weibull Plots
- Miner's Rule
- Coffin-Manson Relation
- Paris' Law
- Gurson Model
- Gurson-Tvergaard-Needleman Model
- Johson-Cook Model
- Structural Fragility Curves
- “Kachanov” Damage Mechanics Models- damage potential surface
- ***They are all based on phenomenological curve fitting techniques. Degradation response is needed before-hand to generate a polynomial.***

Unified Mechanics vs. Newtonian Mechanics

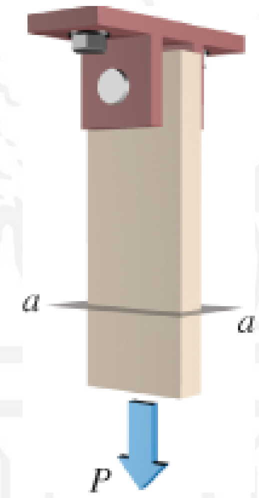
- **Newtonian Mechanics Theory, 1687**
- *Displacement u is the only nodal unknown*
- *"a" & "k" don't change over time*

- $F = ma \quad and \quad F = ku$

- **Unified Mechanics Theory, 1997**
- **Displacement u, and $\dot{\gamma}$ Entropy generation rate are**
- **nodal unknowns.**
- **Stiffness "k", acceleration "a" change continuously.**

- $F = ma\left(1 - \Phi(\dot{s}\,)\right) \; and \; F = ku\,(1 - \Phi(\dot{s}))$

- *no need for curve fitting, or empirical potential/*
- *Or empirical degradation/healing evolution function*



Statistical Mechanics in Boltzmann’s kinetic theory

- **Translation of Ludwig Boltzmann’s Paper** “On the Relationship between the Second Fundamental Theorem of the Mechanical Theory of Heat and Probability Calculations Regarding the Conditions for Thermal Equilibrium” Sitzungberichte der Kaiserlichen Akademie der Wissenschaften. Mathematisch-Naturwissen Classe. Abt. II, LXXVI 1877, pp 373-435 (Wien. Ber. 1877, 76:373-435). Reprinted in Wiss. Abhandlungen, Vol. II, reprint 42, p. 164-223, Barth, Leipzig, 1909
- Kim Sharp * and Franz Matschinsky, Entropy **2015**, 17, 1971-2009; doi:10.3390/e17041971

- Ehrenfest, P. and T. **1911**, **The Conceptual Foundations of the Statistical Approach in Mechanics,** Dover, New York.

- 1934, Swiss physical chemist Werner Kuhn successfully derived a thermal equation of state for rubber molecules using Boltzmann's formula.

- Brush, S. **1983**, **Statistical Physics and the Atomic Theory of Matter, Princeton University Press, Princeton, New Jersey.**

Thermodynamic State Index - Φ

- Let that probability of a material being in a completely ordered ground state is equal to W_o
- . In an alternative configuration, material deviates from this perfectly ordered reference state under actions of external loads (mechanical, **thermal**, electrical, magnetic, **chemical, radiation, corrosion** and **etc.**) to another disordered state with a probability of W.
- $W_o \text{ ------} \rightarrow W$

Irreversible Damage & Healing

- 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 through introduction of damage (change) in system, damage (the measure of change) and entropy (the measure of disorder) are naturally related.

- .

Thermodynamic State Index (TSI), Φ

- In order to relate entropy and *“damage”*, consider a system in ground state $\Phi = 0$ with a total entropy of S_o and an associated probability of W_o .
- In an alternative disordered (“damaged”) state, S is total entropy of the same system with an associated probability of W and a TSI of Φ.
- it is assumed that “damage” can be related to **probability of difference of microscopic configurations** from the ground state probability $\Phi = f(W, W_o)$

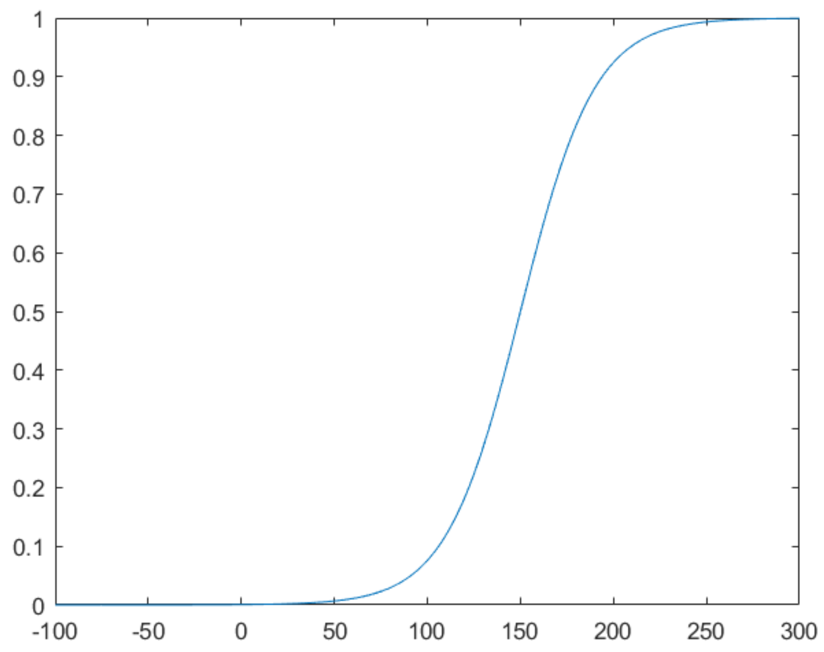
Reference Thermodynamic States

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

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

Universal “Degradation Evolution Function: Thermodynamic State Index (TSI): Φ

- $\Phi = f\left[\frac{W - W_o}{W}\right] = [1 - e^{-\frac{(s - s_o)m_s}{kN_o}}]$



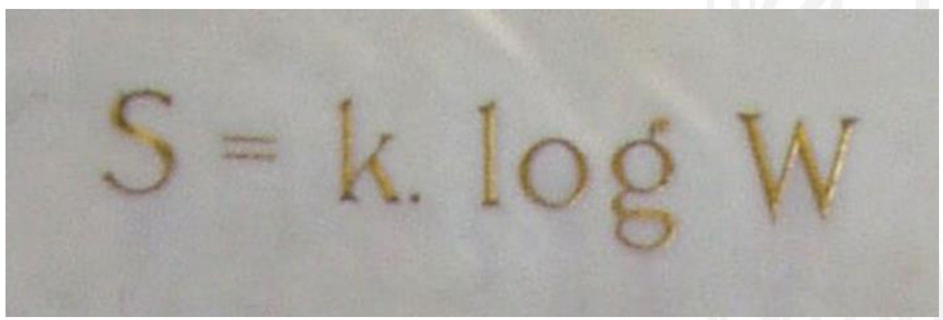
Implementation other Mechanics Theories

- Hamiltonian Mechanics
- Lagrangian Mechanics

- Are implemented in the same fashion since they are all derivatives of Newtonian Mechanics.

2nd Law of Thermodynamics – Entropy Law

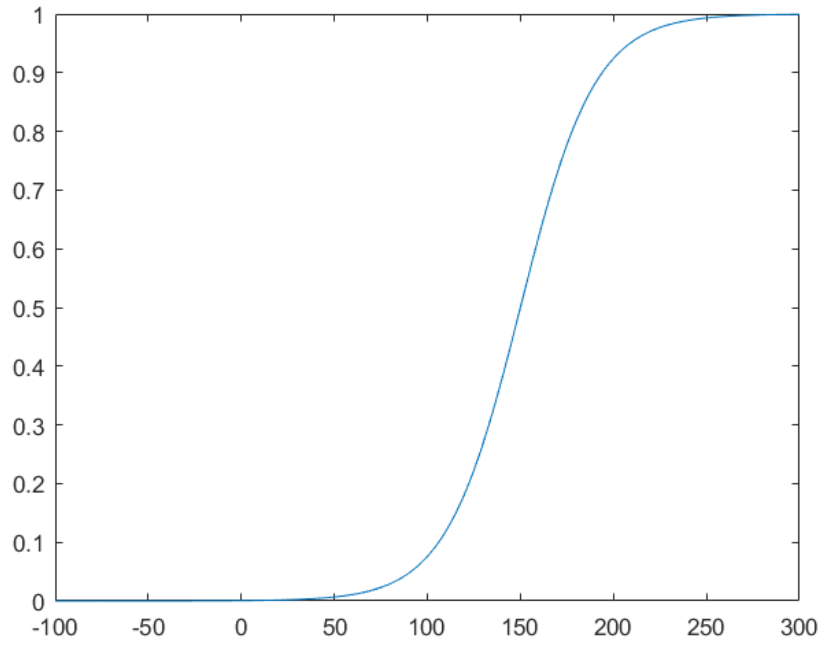
- The Second Law states that there is a natural tendency of any isolated system, living or non-living, to degenerate into a more disordered state. When **irreversible entropy generation rate** becomes zero the system reaches "THE END" (fails/dies).



The logarithmic connection between entropy and disorder probability was first stated by L. Boltzmann (1872) and put into final form by Maxwell Planck (1900) Note that Boltzmann formulates this hypothesis for an arbitrary body, i.e. formulation in the original paper is NOT restricted to gases.

Universal "Degradation" Evolution Function: Thermodynamic State Index (TSI): Φ

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



Entropy Computation does not Require any Curve Fitting Parameters

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

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

Irreversible Entropy Production due to

1- Internal heat generation

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

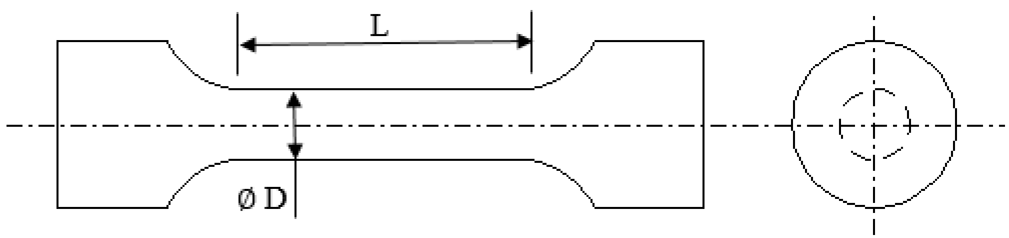
3- Internal mechanical work

Concept first published

- Basaran, C. and Yan, C. Y., **"A Thermodynamic Framework for Damage Mechanics of Solder Joints",** Trans. 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, 3, 205-224, July 2004
- Mathematical Proof
- Sosnovskiy, L.A. and Sherbakov, S.S. **"Mechanothermodynamic Entropy and Analysis of Damage State of Complex Systems"**, Entropy (2016), 18, 268;

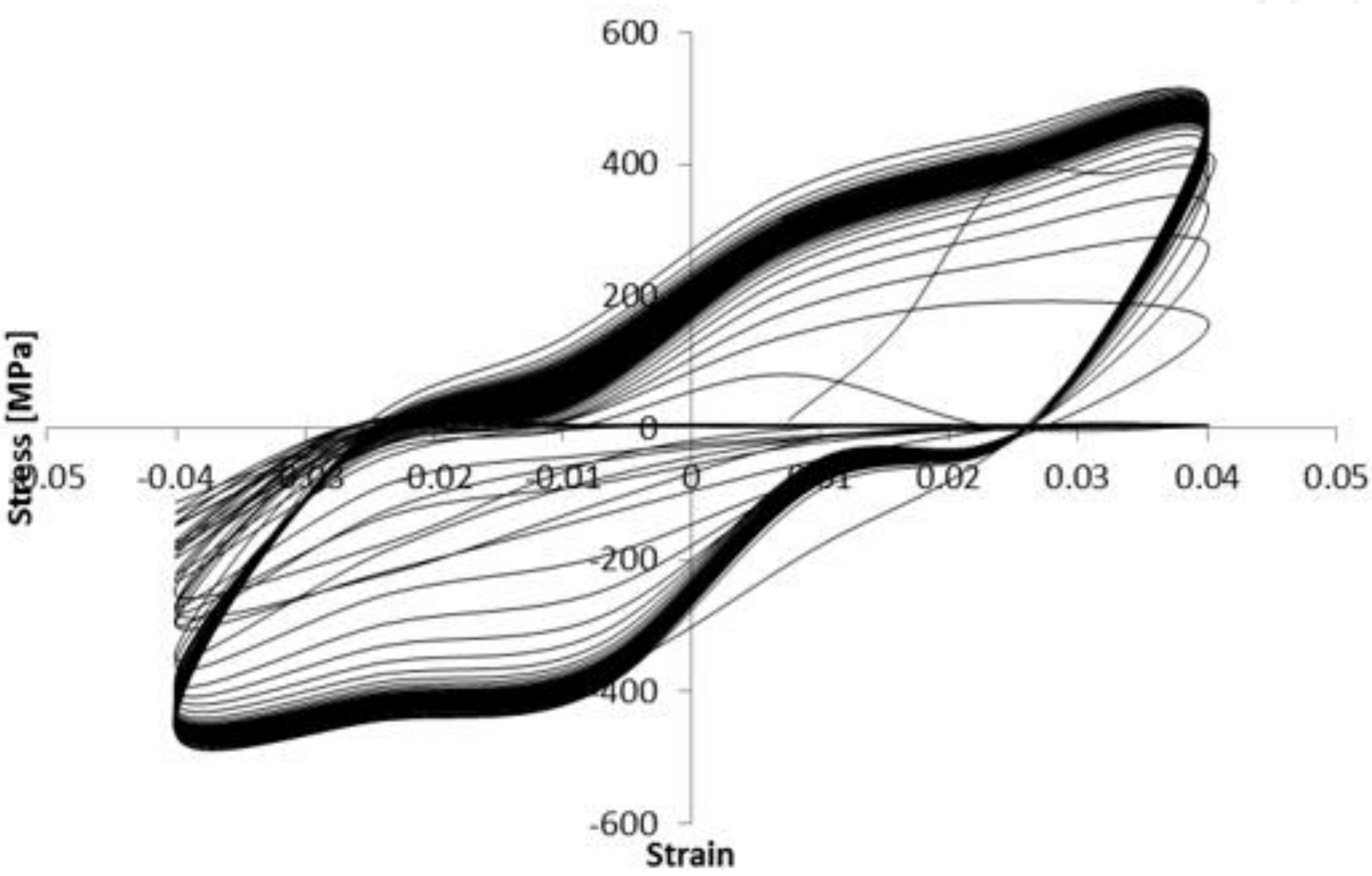
Experimental Verifications

Fatigue Loading on A-36 Steel

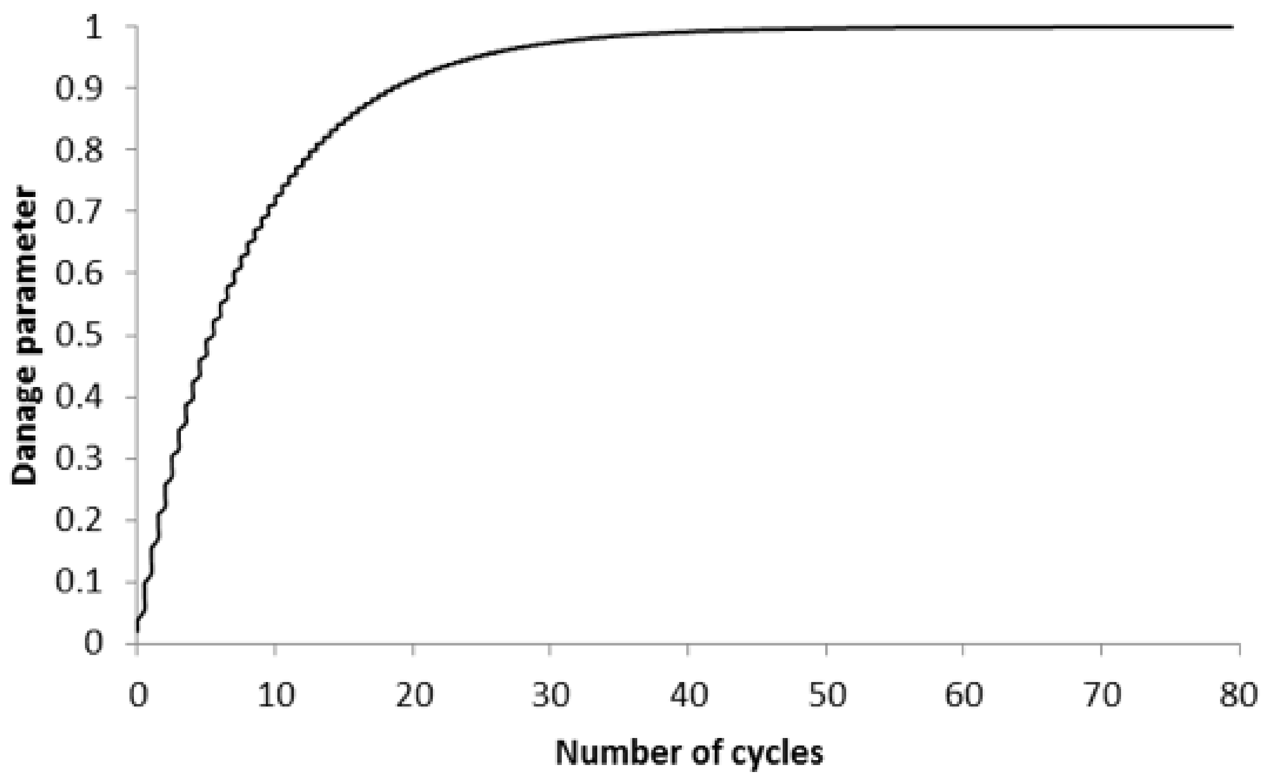


L=25mm	D=6.4mm
E=210000MPa	ν=0.3
T=295K	R=8.314J/K.mol
ρ=7750kg/m^3	m_s=55.8 g/mol

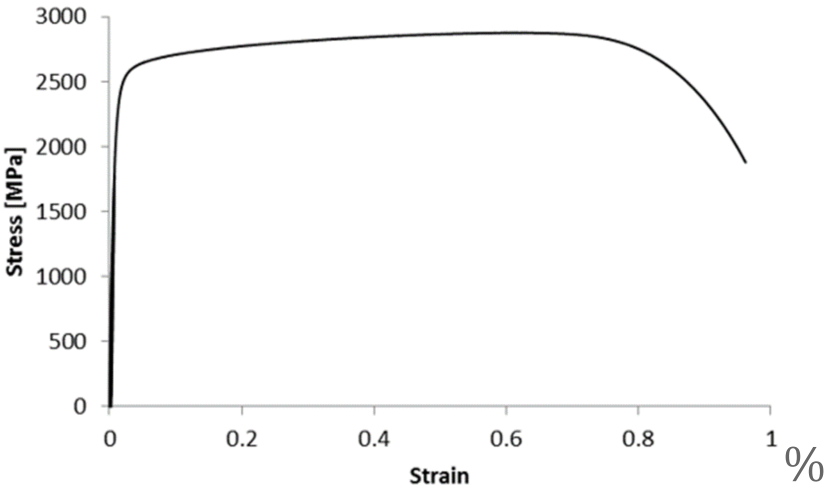
Fatigue Loading – Displacement Controlled Test



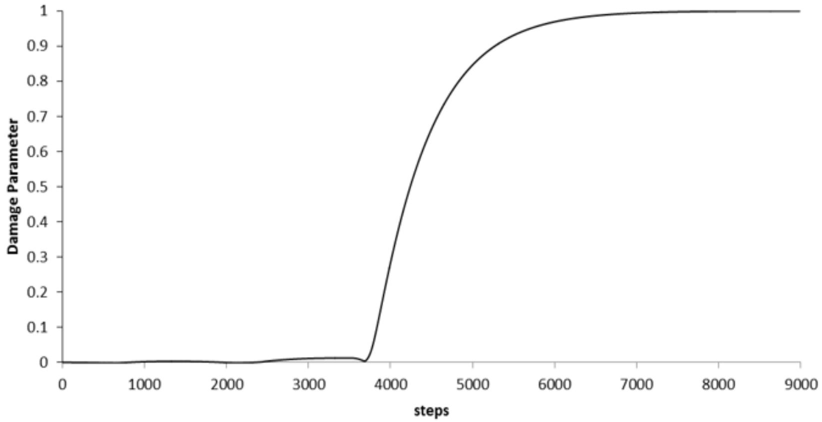
Damage Evolution – Calculated from Experiment



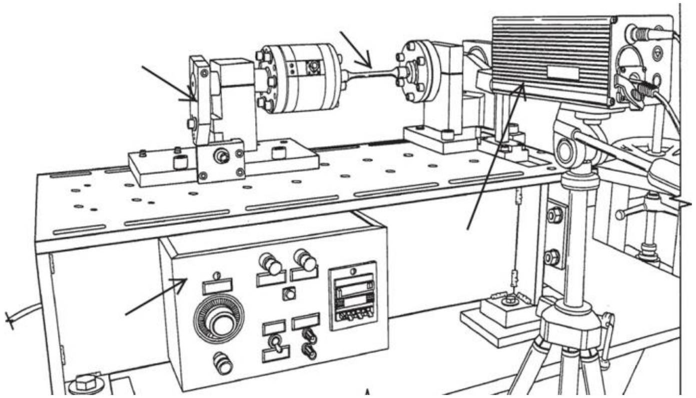
Monotonic Loading Test



Damage - (Thermodynamic State Index)



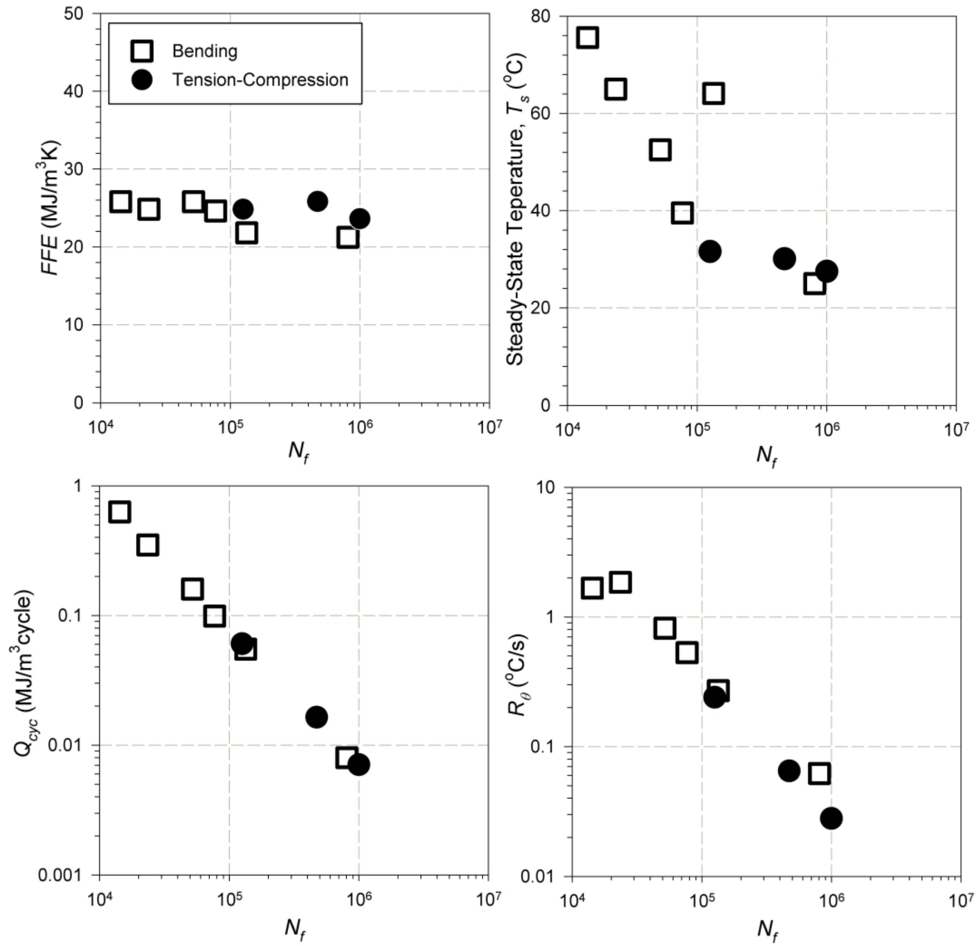
M. Naderi, M. Amiri and M. M. Khonsari , On the thermodynamic entropy of fatigue fracture" **Proceedings of the Royal Society A** (2010) 466, 423–438



"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."

J.Y. Yang and M.M. Khonsari ‘On the Evaluation of Fracture Fatigue Entropy” *Theoretical and Applied Fracture Mechanics*, 2018, in print

Results show that the Fracture Fatigue Entropy remains constant and the fatigue failure prediction using the entropy is independent of the loading condition, frequency, and the geometry.



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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”.

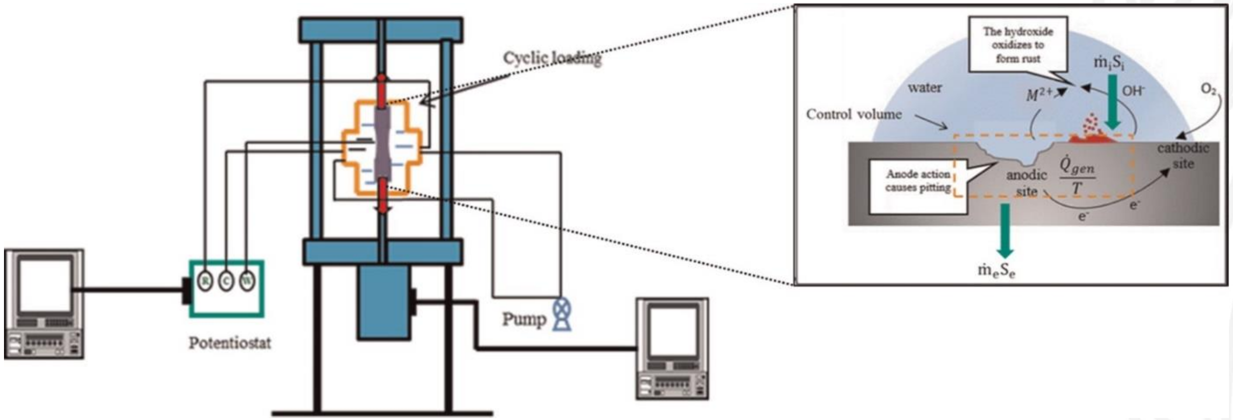
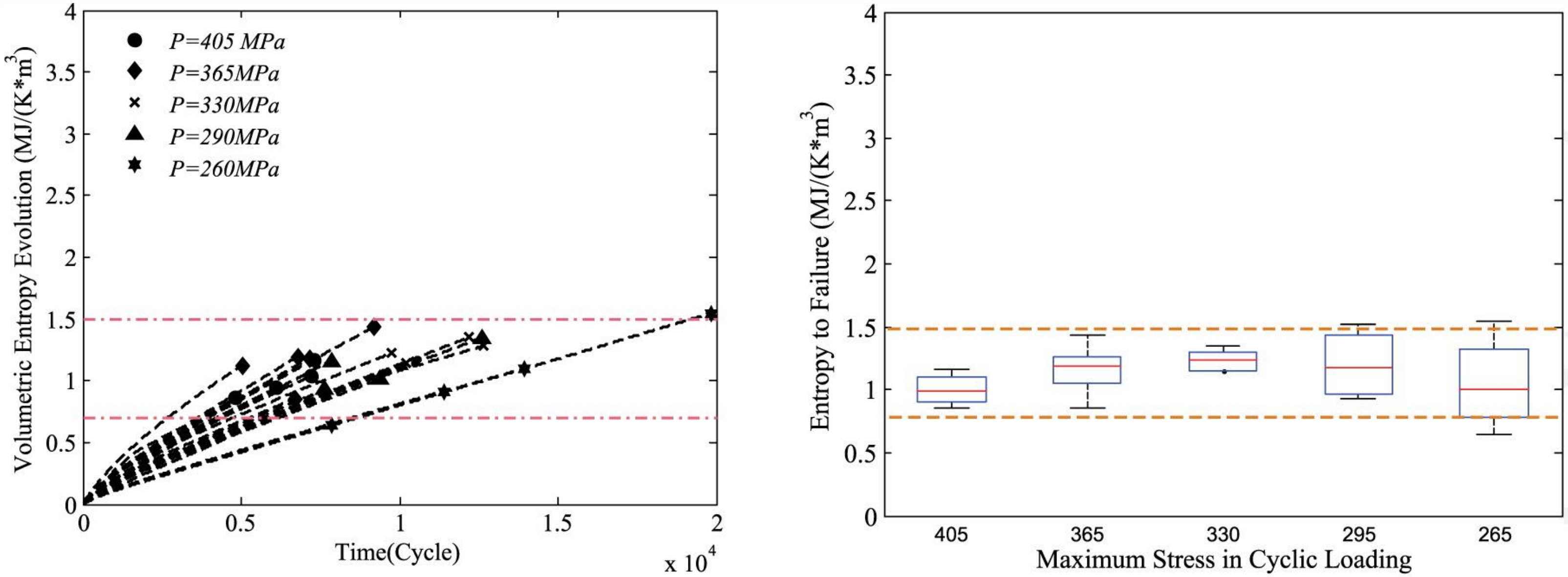


Figure Entropy flow in the control volume under corrosion-fatigue



(a) (b)

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

Imanian, A., Modarres, M., “A Thermodynamic Entropy-Based Damage Assessment with Applications to Prognosis and Health Management”, **Structural Health Monitoring**, 2018, Vol. 17(2) 240–254 DOI: 10.1177/1475921716689561

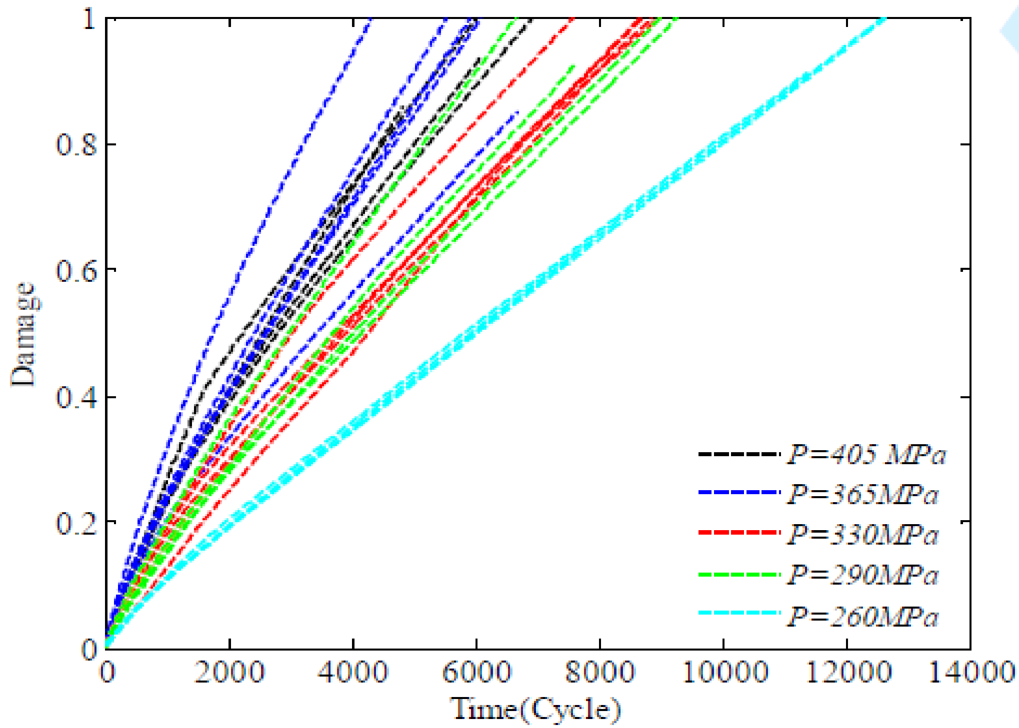
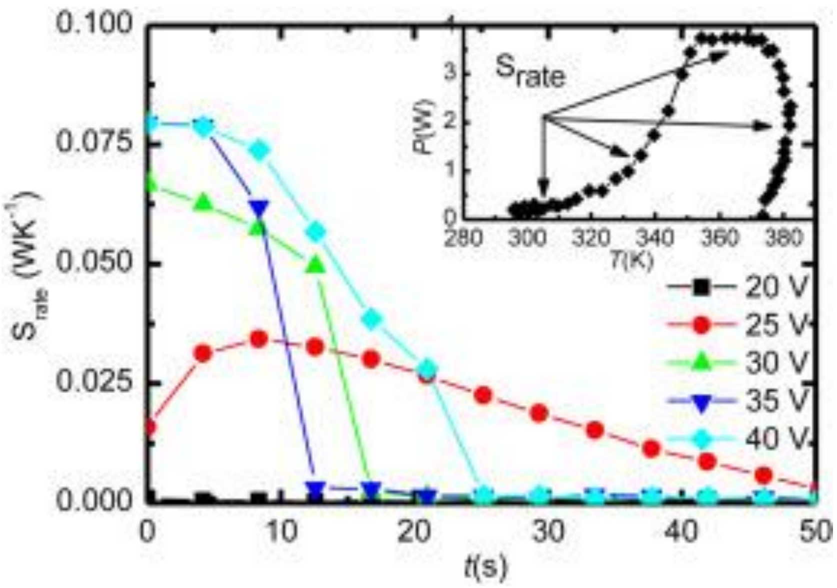


Figure 3. Damage evolution trends

Jundong Wang and Yao Yao" An Entropy Based Low-Cycle Fatigue Life Prediction Model for Solder Materials" *Entropy* **2017**, 19, 503; doi:10.3390/e19100503

Eight groups of experiments were performed under different aging treatment and experiment conditions. The fatigue life predictions agree well with experimental data.

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)

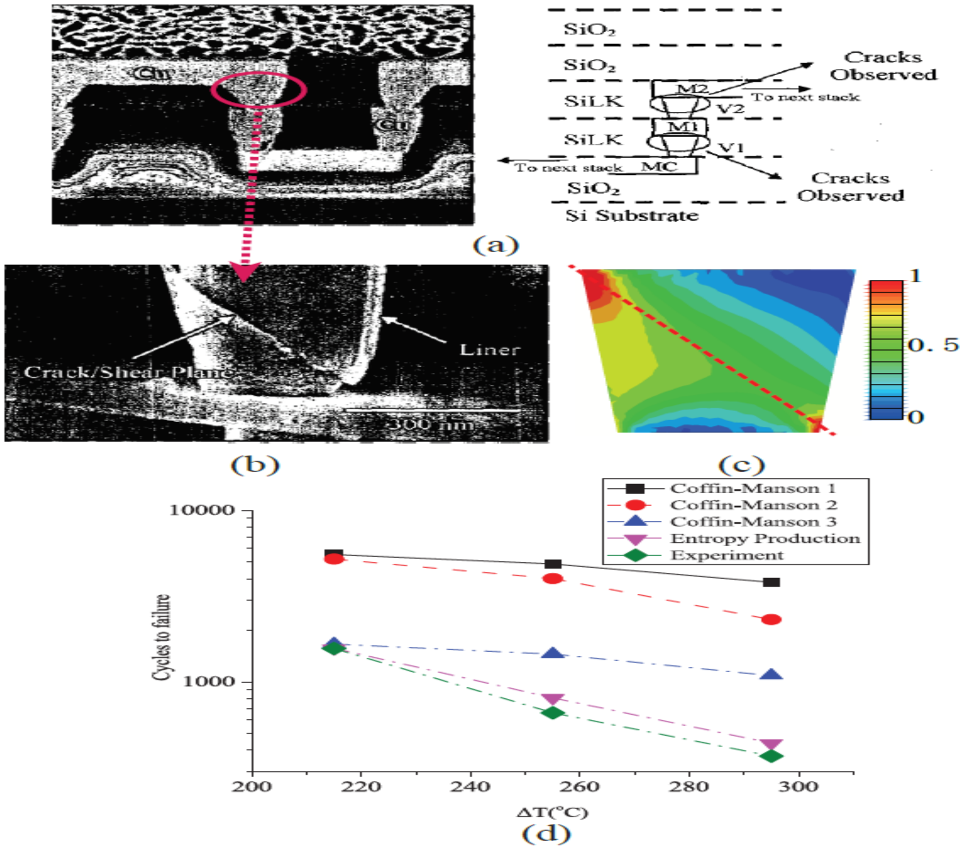
Conclusions

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

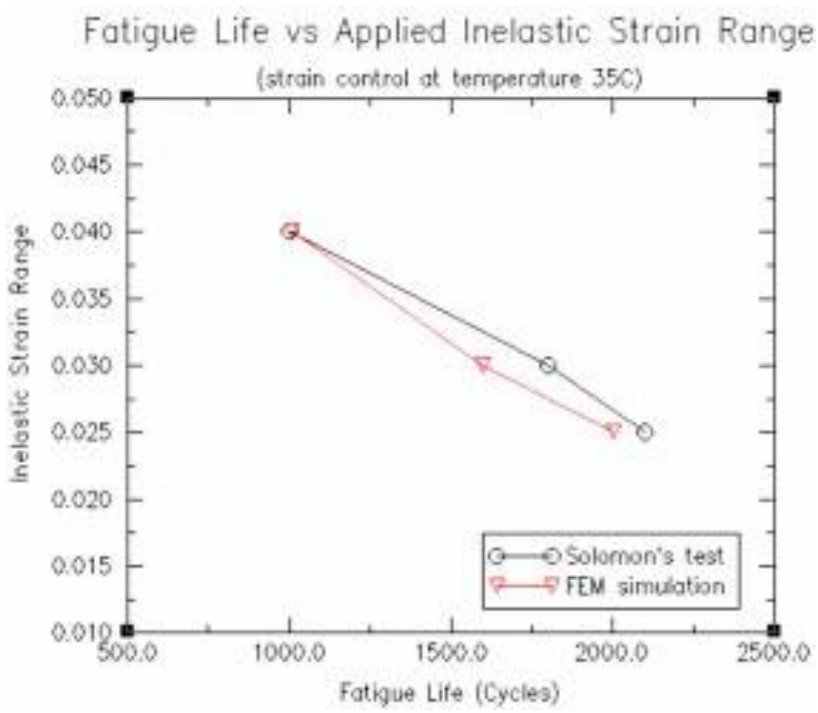
Note: A Light-Emitting Diode is a two-lead semiconductor light source. It is a p–n junction diode that emits light when activated.

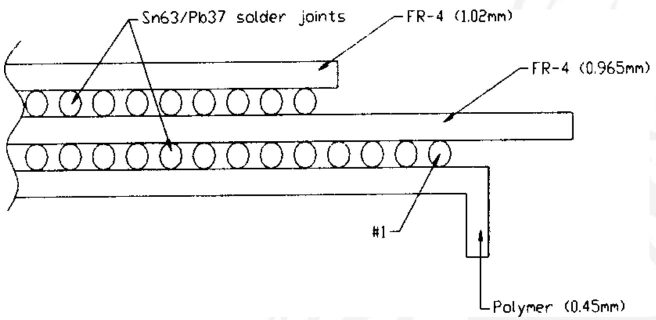
Entropy Production Based Full-Chip Fatigue Analysis: From Theory to Mobile Applications

Tianchen Wang, Sandeep Kumar Samal,Sung Kyu Lim,and Yiyu Shi,
IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems 4/2018. DOI 10.1109/TCAD.2018.2803623



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.

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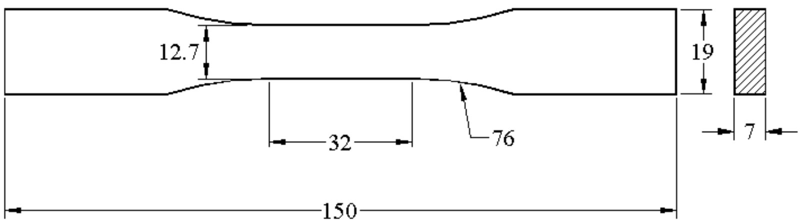
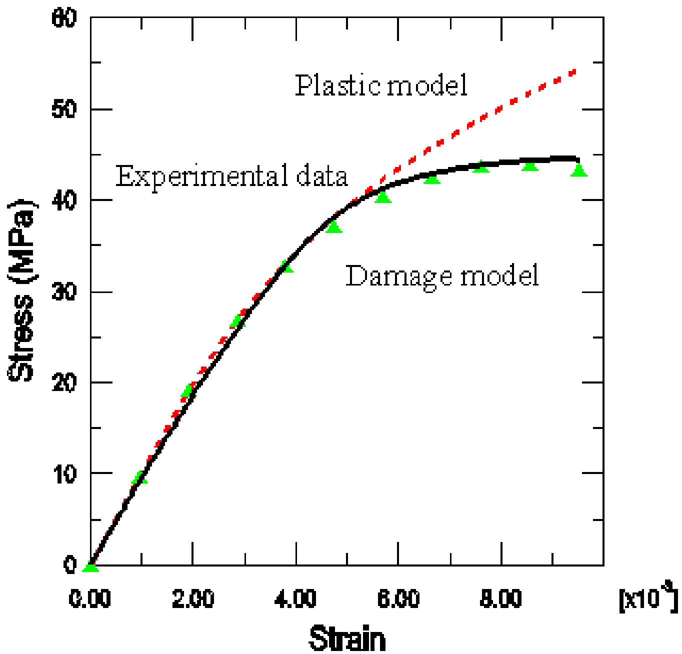
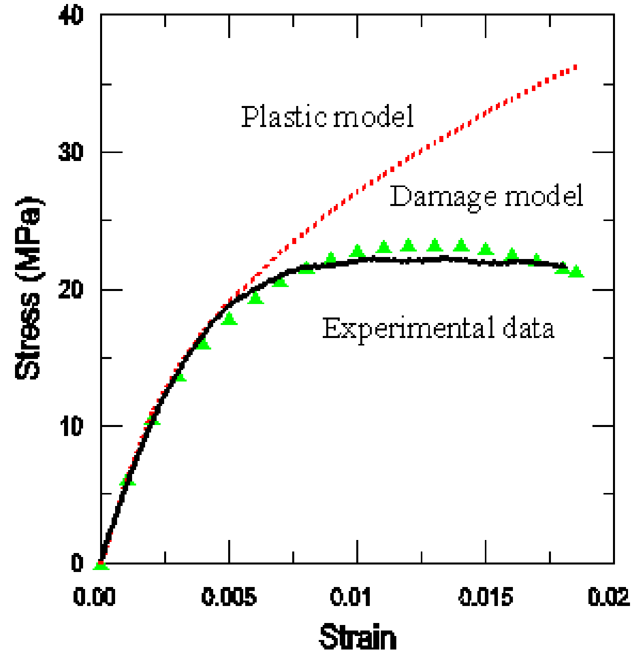
Uniaxial tensile test on Particle Filled Composite



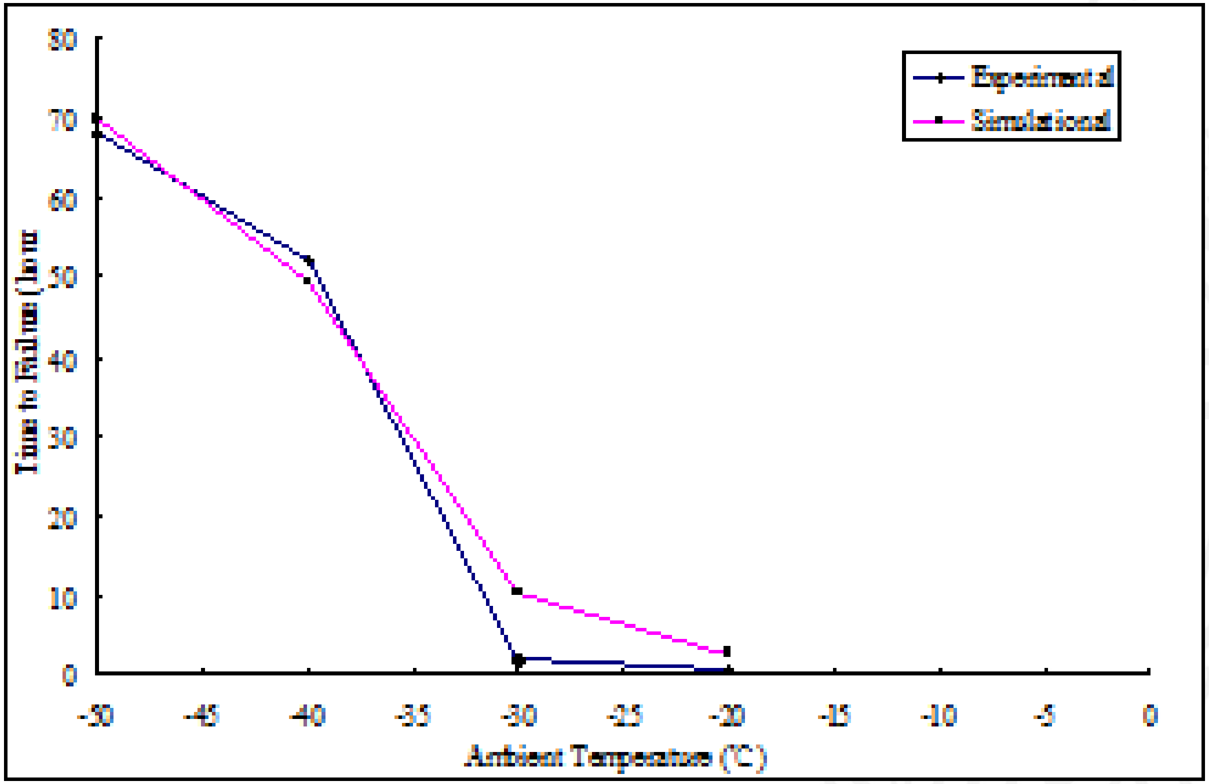




Damage coupled plastic model, Ramberg-Osgood plasticity model and experiment data at 24 ^{0}C and 75^{0} C

Basaran, C. and Nie, S.“A Thermodynamics Based Damage Mechanics Model for Particulate Composites,” International Journal of Solids and Structures, 44, (2007) 1099-1114

Time to Failure under EM + TM for different Ambient Temp



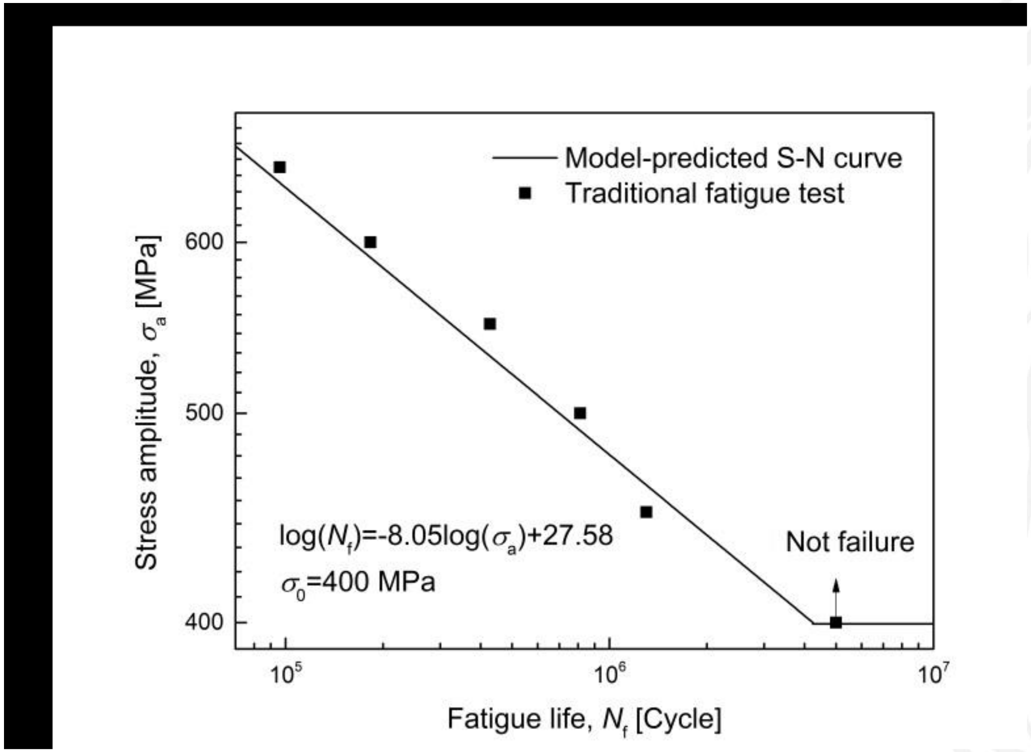
S. Li, M. F. Abdulhamid,and C. Basaran "Simulating Damage Mechanics of Electromigration and Thermomigration," Transactions of the Society for Modeling and Simulation International Vo. 84, No 8/9, pp. 391-401 August/September 2008

Time to Failure : Simulation vs. Test Data

Current Density	Experiment Data $TTF=a/j^3e^{(b/T)}$ (hours)	Simulation Results (D_{cr}=1) (hours)
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

Basaran,C., Li, S., Hopkins, D.C. and Veychard, D. "Electromigration time to failure of SnAgCuNi solder joints“ **Journal of Applied Physics**. 106, 013707 (2009)

Qiang Guo , Fahmi Za¬õri , Xinglin Guo, **An intrinsic dissipation model for high-cycle fatigue life prediction**, *International Journal of Mechanical Sciences (2018) doi:10.1016/j.ijmecsci.2018.02.047*



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CONCLUSIONS

- **Unified Mechanics Theory** replaces **Newtonian Mechanics Theory** to be able to account for actual response of any system.

- **Unified Mechanics Theory** provides a physics based universal degradation evolution function valid under all loading conditions, i.e. Mechanical, Thermal, Chemical, Electrical, Radiation, Corrosion, Magnetic & Others.

- **Assumption:** Everything in the universe is a continuously evolving thermodynamic system.

QUESTIONS