UNIFIED MECHANICS THEORY

Unification of Newtonian Mechanics & Thermodynamics

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Fracture and Lifetime of Materials - In Honor of Prof. Alexander Chudnovsky's 80th Birthday
• Presentation Outline

• I- Objective
• II- Introduction
• III- Literature
• IV- Theory & Mathematical Verifications
• V- Experimental Verifications
• VI- Conclusions
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.
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

  \[ F = ma \quad \text{and} \quad F = ku \]

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

  \[ F = ma \left(1 - \Phi(\dot{s})\right) \quad \text{and} \quad F = ku \left(1 - \Phi(\dot{s})\right) \]

• **no need for curve fitting, or empirical potential/**
• **Or empirical degradation/healing evolution function**
Statistical Mechanics in Boltzmann’s kinetic theory


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

Thermodynamic State Index - $\Phi$

- 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 $W$.

\[ W_o \quad \rightarrow \quad W \]
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), $\Phi$

- 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 $\Phi$.
- 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, $W_{\text{max}}$. At this stage, entropy production rate will become zero. TSI will be maximum $\Phi = 1$. 
Universal “Degradation Evolution Function: Thermodynamic State Index (TSI): $\Phi$

$$\Phi = f \left[ \frac{W - W_0}{W} \right] = \left[ 1 - e^{-\frac{(s - s_0)m_s}{kN_0}} \right]$$
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).

\[ S = k \log W \]

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): $\Phi$

$\Phi = f \left[ \frac{W - W_o}{W} \right]$
Entropy Computation does not Require any Curve Fitting Parameters

\[ \Delta s = \int_{t_0}^{t} \frac{1}{\rho} \dot{s} \, dt \]

\[ \Delta s = \int_{t_0}^{t} \left\{ \frac{1}{\rho T^2} k_T |\text{Grad}(T)|^2 + \frac{r}{T} + \frac{C_v D_{\text{effective}}}{\rho k_B T^2} \left[ Z_i e \rho^* j - f \Omega \nabla \sigma_{\text{spherical}} + \frac{Q^* \nabla T}{T} + \frac{k_B T}{c} \nabla C \right]^2 \right\} \, dt \]

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


• Mathematical Proof

Experimental Verifications
Fatigue Loading on A-36 Steel

\[ L = 25\text{mm} \quad E = 210000\text{MPa} \quad T = 295\text{K} \quad \rho = 7750\text{kg/m}^3 \]

\[ D = 6.4\text{mm} \quad \nu = 0.3 \quad R = 8.314\text{J/K.mol} \quad m_r = 55.8\text{ g/mol} \]
Fatigue Loading – Displacement Controlled Test
Damage Evolution – Calculated from Experiment
Monotonic Loading Test

Damage - (Thermodynamic State Index)

“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.”

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.

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


Figure 3. Damage evolution trends
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. Ovejas

Entropic characterization of overstressed capacitors for lifetime prediction, 
*Journal of Power Sources*, Volume 336, 30 December 2016, Pages 272–278

“...proposed a method to estimate ageing in electrolyte capacitors based on a measurement of entropy generation rate, $S_\text{rate}$.”

Time evolution of entropy generation rate $S_\text{rate}$ and capacitance for the capacitor
33 mF capacitor biased with a 4 V pulsed excitation.
Angel Cuadras, Jiaqiang Yao, and Marcos Quilez,” Determination of LEDs degradation with entropy generation rate” 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.
Entrophy Production Based Full-Chip Fatigue Analysis: From Theory to Mobile Applications

Fatigue due to Temperature Cycling

Uniaxial tensile test on Particle Filled Composite

Time to Failure under EM + TM for different Ambient Temp

### Time to Failure: Simulation vs. Test Data

<table>
<thead>
<tr>
<th>Current Density</th>
<th>Experiment Data TTF=a/j^3e^{(b/T)} (hours)</th>
<th>Simulation Results (D_{cr}=1) (hours)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0 \times 10^4 Amp/cm²</td>
<td>228.7</td>
<td>222.41</td>
</tr>
<tr>
<td>0.8 \times 10^4 Amp/cm²</td>
<td>446.6</td>
<td>435.33</td>
</tr>
<tr>
<td>0.6 \times 10^4 Amp/cm²</td>
<td>1058.7</td>
<td>1098.2</td>
</tr>
</tbody>
</table>

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