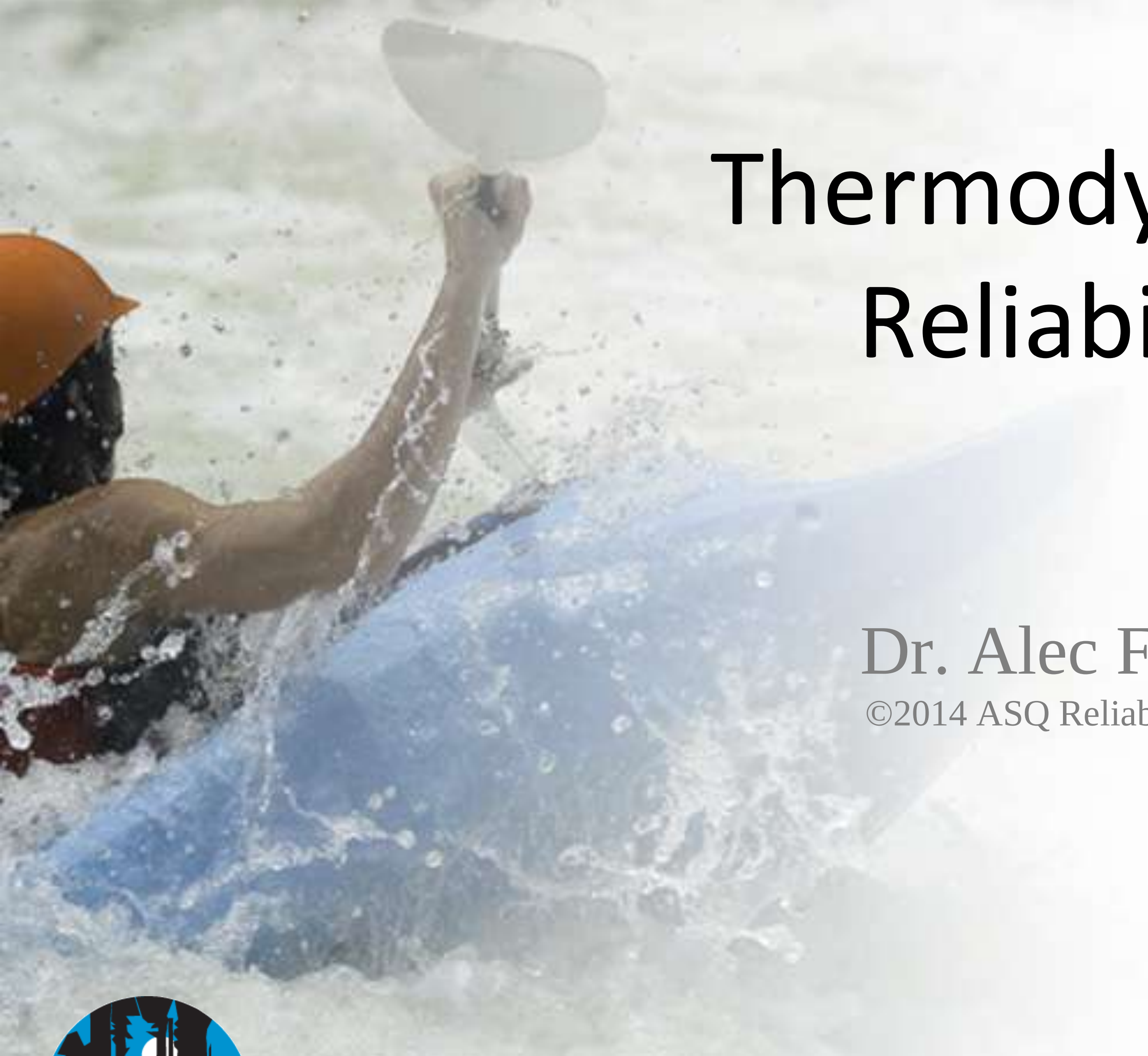

Thermodynamic Reliability

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ASQ Talk Thermodynamic Reliability

For ASQ members the **video** and the slides are also available at:

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Equations in this talk are incorporated in DfRSoft software described at the website

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NEW BOOK: Only reference for this material

The Physics of Degradation in Engineered Materials and Devices

Editor: Dr Jonathan Swingler, Heriot-Watt University, England

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Published by: Momentum Press

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Book Overview:

The Physics of Degradation in Engineered Materials and Devices

- **Chapter 1:** Introduction, Dr Jonathan Swingler
- **Chapter 2:** The History of the Physics of Degradation, Dr Jeffrey Jones,
- **Chapter 3:** Thermodynamics of Engineering, Prof Michael Bryant
- **Chapter 4: Thermodynamic Damage within Physics of Degradation, Dr Alec Feinberg**
- **Chapter 5:** Monitoring Degradation in the Field., Dr Xiandong Ma,
- **Chapter 6:** Physics of Degradation in Polymers Electronics, Prof Hari et al
- **Chapter 7:** Physics of Degradation in Ferroelectric Devices,Prof Paul Weaver

What is Thermodynamic Reliability?

- A relatively new evolving science – now being recognized at the university level
- It merges thermodynamics with reliability
- It can help
  - Understand why materials degrade
  - Lead to new ways to make better and more meaningful measurements
  - Help in the making of new materials
  - Provide new approaches to solving and detecting degradation
  - Can be used at the system and component level
- “To overlook the potential this science has in its ability to contribute to reliability physics would be a mistake”

Thermodynamics: a fundamental Science for Physics-of-failure

- Thermodynamics Second Law can be used to describes aging damage
  - ***Second law in terms of device thermodynamic damage:*** *The spontaneous irreversible damage processes that take place in a <u>device</u> interacting with its <u>environment</u>, do so in order to go towards <u>thermodynamic equilibrium with its environment</u>.*

Examples

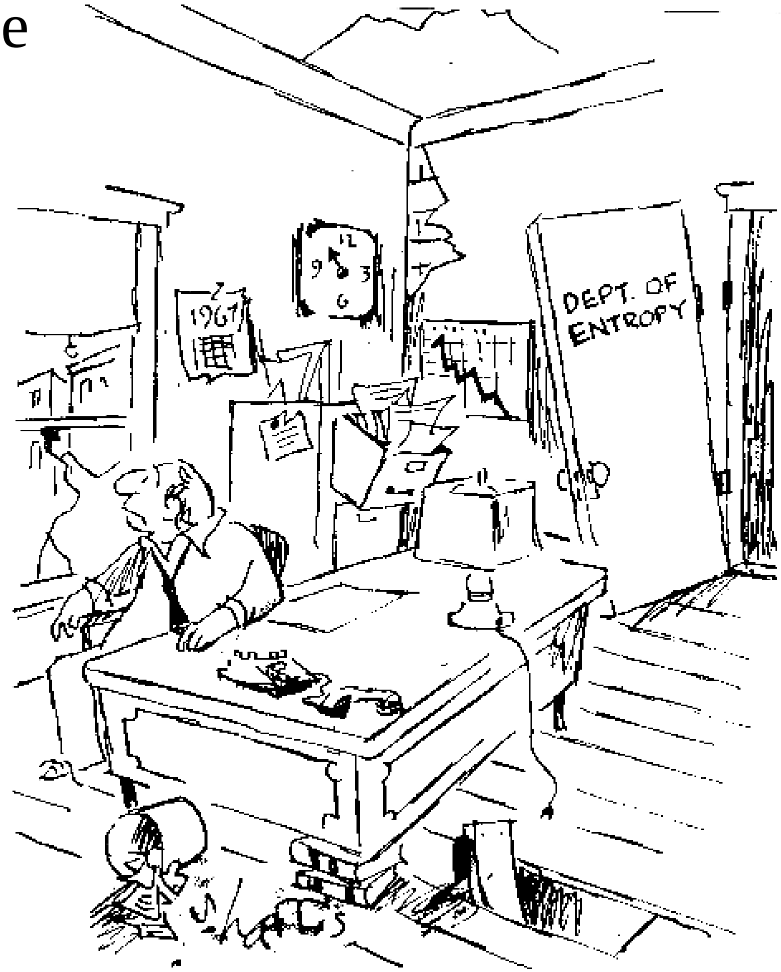
- Semiconductor component, steel beam, or a bicycle tire
- Each system interacts with its environment
- The interaction between the system and environment degrade the system in accordance with our second law
- Degradation is driven by this tendency of the system/device to come into thermodynamic equilibrium with its environment
- Air in bike tire will deflate, steel beam will rust/corrode, semiconductor diffusion will start to occur

Order in the System Decreases Causing Damage

- Total order of the system plus its environment tends to decrease
- The spontaneous processes creating disorder are irreversible
- Air will not go back into the bike tire
- Semiconductor will not spontaneously purify
- Steal beam will continue to corrode
- The original order created in a manufactured product diminishes in a random manner, and becomes measurable

Assessing Damage in Equilibrium Thermodynamics

- Thermodynamic state variables define the equilibrium state of the system
- State variables examples:
  - temperature, volume, pressure, energy, entropy, mass, voltage, current, electric field, vibration displacements...
- **Entropy or Free Energy** are key variables to help assess damage



Damage Causes a Loss of Ability to do Useful Work

- Disorder is associated with device damage
- Entropy change measures damage
- If entropy does not increase, there is no degradation
- Not all entropy increase causes damage
- Adding or removing heat, increase or decrease entropy. Yet device damage may not occur
- Heating a transistor does not always cause permanent damage. We can put air back in the tire but we cannot repair a corroded steel beam.

Entropy Damage

- *The entropy generated associated with device damage, is, **“entropy damage”***
- ***Entropy Generated*** $\boldsymbol{S_{gen}}$
  - $S_{gen}=\Delta S_{total}=\Delta S_{device}+\Delta S_{env}\geq 0$
- ***We can write entropy change in terms of the Non Damage and Damage?***
  - $\Delta S_{device}=\Delta S_{damage}+\Delta S_{non\text{-}damage}\geq 0$

Measuring Entropy Damage

- *Devise a gentle measurement process "f", to measure entropy change in a time period Δt.*
  - *Make an initial measurement at time t_1*
  - $\Delta S_f(t_1) = S(t_1 + \Delta t) - S(t_1)$ *time* t_1
  - *Expose the device to aging until time t_2 then make a 2^{nd} measurement*
  - $\Delta S_f(t_2) = S(t_2 + \Delta t) - S(t_2)$, *where* $t_2 >> t_1$
- Entropy damage:

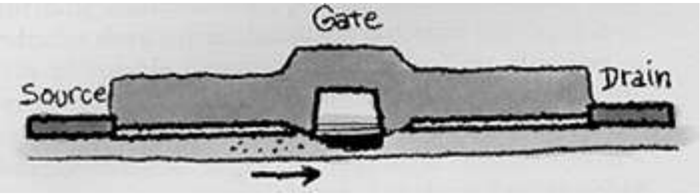
$$\Delta S_{f\text{-}Damage}(t_2,t_1) = \Delta S_f(t_2) - \Delta S_f(t_1) \geq 0$$

  - Note: Equal to 0 => no Damage

Measuring Entropy Damage (Cont.)

- We can also look at the aging ratio

  Aging Ratio= $\Delta S_f(t_1) / \Delta S_f(t_2)$ *what is an acceptable % ??*
- Note the measurement process itself should not cause significant damage compared to aging damage
- Aging stress must be limited to within reason so that we can repeat our measurement in a consistent manner.
- See Selected Examples



Complex Systems Entropy Damage

- The total entropy of a system is equal to the sum of the entropies of the parts. If we isolate an area enclosing the system and its environment such that no heat, mass flows, or work flows in or out, then the entropy generated is

$$S_{Gen} = \Delta S_{Total} = \sum_{i=1}^{N} \Delta S_i = \Delta S_{Sys} + \Delta S_{Surroundings} \geq 0$$

- ***This is an important result for thermodynamic damage***. If we can keep tabs on ΔS_{Total}

over time, we can determine if aging is

occurring even in a complex system.

- See Selected Examples

Selected Results in Equilibrium Thermodynamics

Example 1 & 2

- *Simple Resistor Aging*

$$\Delta S_{Damage}(t_2,t_1)=mC_{p-avg}Ln\frac{T_4}{T_3} \qquad A_{Aging-ratio}=Ln(T_3/T_2)/Ln(T_4/T_2)$$

- Where $C_{p\text{-}Avg}$ average specific heat of resistor, m=resistor mass, T_2 room temperature
- Time t_1:T_3 temp. rise when current I_1 passes through
- Time t_2 (Month Later): T_4 temp rise when current I_1 passes through it

- *Example 2: Complex but similar Resistor Bank to Ex 1*

$$A_{Aging-ratio}=Ln(T_3/T_2)/Ln(T_4/T_2)$$

Example 3

- *System of similar parts (incompressible constant volume)*

$$\Delta S_{Total} = \sum_{i=1}^{N} \Delta S = (\sum_{i=1}^{N} m_i C_{Avg\ i})(Ln \frac{T_2}{T_1})$$

- Where C_{Avgi} average specific heat of parts, m_i= mass

$$A_{Aging-ratio} = Ln(T_3/T_1)/Ln(T_2/T_1)$$

At Initial Time

T_1=Initial Temperature of System

T_2=T_1+Temperature rise of system in operation initially

At a time later when aging has occurred

T_1=Initial Temperature of System

T_3=T_1+Temperature rise of system in operation at later time

Numeric Example 4

- Prior to a system being subjected to a harsh environment, we make an initial measurement M1$^+$ at ambient temperature. Then the system is subjected to an unknown harsh environment. We then return the system to the lab and make a measurement M2$^+$ in the exact same way that M1 was made. Find the aging ratio where
  - M1: $T1=300^oK$, $T2=360^oK$,
  - M2: $T1=300^oK$, $T3=400^oK$

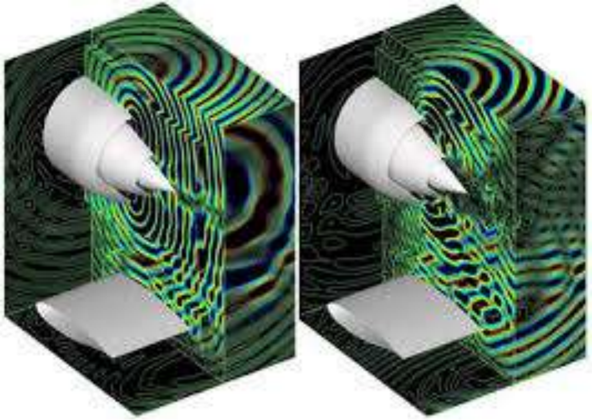
Solution:

$$A_{Aging-ratio} = Ln(400/300)/Ln(360/300) = 1.58$$

System has aged by a factor of 1.58. We next need to determine what aging ratio is critical.

+ Note: In the strict thermodynamic approach M1 and M2 should be made with the system thermally insulated. However, if we can make a measurement in a repeatable way say with a thermal couple on a specific surface of interest we should get reasonably accurate results.

Example 5



- Noise can be considered a system level state variable
- Noise Degradation of isolated system and environment with system exhibiting **white noise** – Thermodynamic entropy analysis results show noise variance is a key state variable

$$\Delta S_{Damage} = S_{t2}(X) - S_{t1}(X) = \Delta S(t2,t1) = \frac{1}{2}\log(\frac{\sigma_{t2}^{2}}{\sigma_{t1}^{2}})$$

- Where
  - At Initial Time
    - $\sigma_{\text{t-initial}}$=Initial standard deviation of white noise
  - At a time later when aging has occurred
    - $\sigma_{\text{t-final}}$=Final or later time value of the standard deviation of white noise

Numeric Example 6

- Prior to a system being subjected to a harsh environment, we make an initial measurement M1^{+} of an engine vibration (fluctuation) profile. Then the system is subjected to an unknown harsh environment. We then return the system to the lab and make a measurement M2 $^{+}$ in the exact same way that M1 was made. Find the aging ratio where
  - M1: Engine exhibits a constant PSD characteristic of 3Grms in the bandwidth from 10 to 500 Hz
  - M2: Engine exhibits a constant PSD characteristic of 5Grms in the bandwidth from 10 to 500 Hz

System noise damage ratio is then: (note variance=Grms for white noise

$$Damage_{noise\_ratio} = Log(5^2)/Log(3^2) = 1.47$$

Assessing Damage in Non Equilibrium Thermodynamic

Equilibrium thermodynamics provides methods for describing the initial and final equilibrium system states, without describing the details of how the system evolves to final state. While, non-equilibrium thermodynamics describes in more detail what happens during the evolution to the final equilibrium state.

Assessing Damage in Non Equilibrium Thermodynamic

- Here we are concerned with the aging path. How does aging occur over time as opposed to just assessing the system’s state at any time point.
- We can use the prior method and sample more to trace out an aging path
- However, using this method, we need to keep track and measure a number of states throughout the aging process.
- Often we are able to model the degradation (damage) so we do not have to make many measurements.

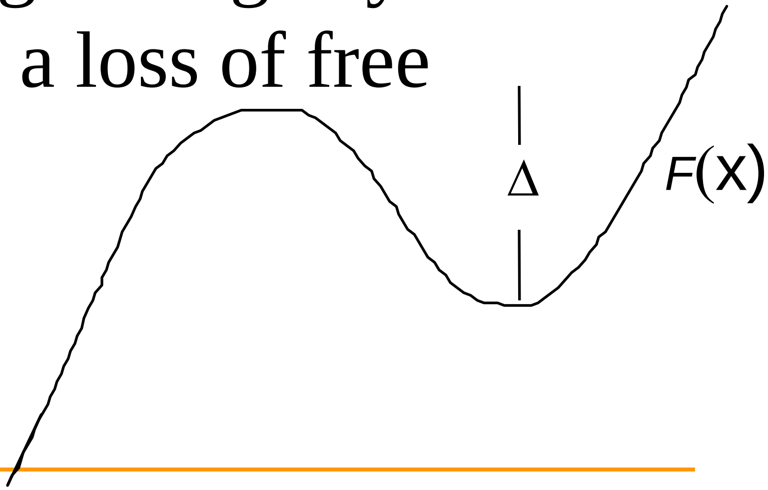
Conjugate Work & Free Energy Approach

- The work done on the system by the environment has the form

$$\delta W = \sum_{a} Y_a \, dX_a \ \text{ or } \ W = \int_{X_1}^{X_2} Y \, dX$$

- Associated with work causing damage by the environment on the device is a loss of free energy F

$$Work = (F_{final} - F_{initial})$$



Damage: Entropy Increases or Free Energy Decreases

- Non Equilibrium Thermodynamics ⟶ Aging State

$$\frac{dS_{Total}}{dt} > 0 \qquad \frac{d\Phi}{dt} < 0$$

Entropy definition

Free energy definition

- Equilibrium Thermodynamics ⟶ Non Aging State

$$\frac{dS_{Total}}{dt} = 0 \qquad \frac{d\Phi}{dt} = 0$$

Entropy is as large as possible

Free energy is as small as possible

Conjugate Work Variable

- Some common thermodynamic work systems

Common Systems **δW**	**Generalized force** **Y**	**Generalized Displacement** **X**	**Mechanical Work** **$\delta W=YdX$**
Gas	Pressure (-P)	Volume (V)	$-P\,dV$
Chemical	Chemical Potential (μ)	Molar number of atoms or molecules (N)	$\mu\,dN$
Spring	Force (f)	Distance (x)	$f\,dx$
Mechanical Wire/Bar	Tension (J)	Length (L)	$J\,dL$
Mechanical Strain	Stress (σ)	Strain (e)	$\sigma\,de$
Electric Polarization	Polarization (-p)	Electric Field (E)	$-p\,dE$
Capacitance	Voltage (V)	Charge (q)	$V\,dq$
Induction	Current (I)	Magnetic flux (Φ)	$Id\Phi$
Magnetic Polarizability	Magnetic Intensity (H)	Magnetization (M)	$H\,dM$
Linear System	Velocity (v)	Momentum (m)	$v\,dm$
Rotating Fluids	Angular velocity (ω)	Angular momentum (L)	ωdL
Resistor	Voltage (V)	Current (I)	$\int VI\,dt$

Thermodynamic Damage Ratio Method for Tracking Degradation

- Total work – some work cause damage and some work is due to damage inefficiencies unrelated to system work damage. In theory we can track the true damage, the types of damage

$$Damage = \frac{\sum_{i=1}^{m} w_{d\,i}}{W_d} \quad and \quad Effective\ \ Damage = \frac{\sum_{i=1}^{m} w_{T\,i}}{W_T}$$

- ***The work damage ratio:*** *This consists of the work performed to the work needed to cause system failure. In system failure, we exhaust the maximum amount of useful system work.*
- *All work found must be taken over the*

same work path.

Damage Ratio (Cont.)

- Cyclic damage can be written over n cycles as

$$Damage = \frac{\dfrac{\sum \oint Y_n dX_n}{n}}{W_{Failure}} = \frac{Partial\ cyclic\ work}{Total\ cyclic\ work\ to\ cyclic}$$

- Non cyclic damage

$$Damage = \frac{\int Y dX}{W_{Failure}} = \frac{Partial\ work}{Total\ work\ needed\ \ for\ \ failure}$$

Same Work Path

Determining Acceleration Factors Using Damage Ratio

- When the degradation path is separable for time

$$w=\int_{t_i}^{t_f} Y(t)\frac{dX(t)}{dt}\,dt = f(Y,k,E_a)\,t$$

- Damage between two different environmental stresses Y_1 and Y_2, and failure occurs for each at time t_1 and t_2 then the damage value of 1 requires that

$$Damage = \frac{f(Y_2,k,E_a)\ \tau_2}{f(Y_1,k,E_a)\ \tau_1} = 1 \qquad or \qquad AF(1,2) = \frac{\tau_2}{\tau_1} = \frac{f(Y_1,k,E_a)}{f(Y_2,k,E_a)}$$

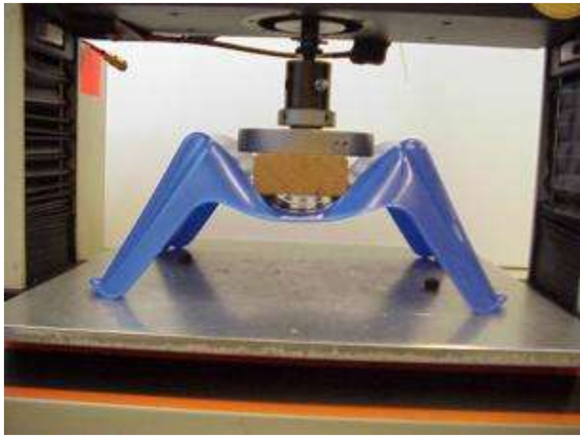
- Then damage can be written (τ_2 AF τ_1)→

$$Damage = \frac{f(Y_1,k,E_a)\ t_1}{f(Y_2,k,E_a)\ \tau_2} = \frac{f(Y_1,k,E_a)\ t_1}{f(Y_2,k,E_a)\,AF(1,2)\ \tau_1}$$

Selected Results in Non Equilibrium Thermodynamics

- Ex. 7: Creep (σ is mechanical stress , ε_p strain)

$$w = \int \sigma \, d\varepsilon_P = \int \sigma \frac{d\varepsilon_P}{dt} dt = \int B\sigma^{M+1} p t^{p-1} dt = B(T)\sigma^{M+1} t^p$$



$$Damage = \sum_i \left(\frac{t_i}{\tau_i} \right)^p = \sum_i \left(\frac{t_i}{AF(1,i)\,\tau_1} \right)^p$$

$$AF = \left(\frac{\tau_c}{\tau_1} \right) = \left[e^{E_a / K_B (\frac{1}{T_1} - \frac{1}{T_2})} \left(\frac{\sigma_1}{\sigma_2} \right)^{-(M+1)} \right]^{1/p}$$

Selected Results in Non Equilibrium Thermodynamics

- Ex. 8: Mechanical Abrasive Wear (non temperature stress related)

$$w = \int F\,dx = \int F \frac{dD}{dt}dt = \int \frac{kP^2\nu}{HA}dt = \frac{kP^2\nu\,t}{HA}$$

$$Damage = \sum_i \left(\frac{t_i}{\tau_i}\right) = \sum_i \left(\frac{t_i}{AF(1,i)\,\tau_1}\right)$$

$$AF(2,1) = \left(\frac{\tau_2}{\tau_1}\right) = \frac{A_2}{A_1}\frac{\nu_1}{\nu_2}\left(\frac{P_1}{P_2}\right)^2$$

V=removed volume of the softer material, *P*=normal load (lbs), *L* is the sliding distance (feet), *H*=hardness of the softer material in psi, wear volume *V*=*AD* where *A* is the area and *D* is the depth of the removed. Then writing $L=\nu t$ for two sliding surfaces rubbing against each other at a constant velocity ν, τ failure time.

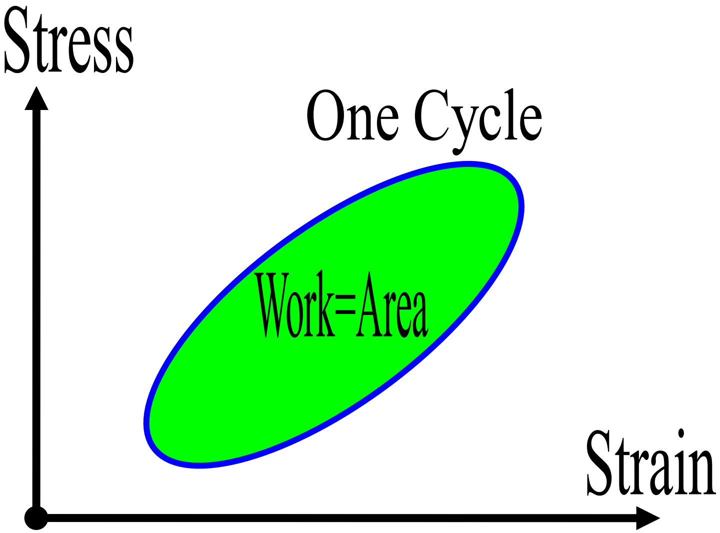
Cyclic Work – How Much Damage/Cycle?

- Cyclic Work cause damage each cycle (Compress-Decompress)
- To estimate the amount of damage we first need to find the total amount of cyclic work done (i.e. the sum of all the cyclic work performed for each cycle)
- For stress and strain type cyclic work the total work is given by

$$w(\text{cycle}) = \sum_{i=1}^{n} \oint_{Area_i} S\,de$$

- The damage is the ratio

$$Damage = \frac{\sum_{i=1}^{n} \oint_{Area_i} S\,de}{W_{Failure}} = \frac{Sum\ work\ per\ cycle}{Total\ work\ needed\ for\ failure}$$



Fatigue Damage Using Miner’s Rule

- Miner’s rule is a popular approximation for finding damage
- Work W is a function of the cyclic area. Miner’s empirically figured that stress S, cycles n were the main factors for damage
    - In our framework this means $W_n=W(S, n)$
- Miner also empirically assumed that the work for n cycles of the same cyclic size is all that is needed – in our framework this means
    - $W_n= n\,W(S)$ (Miner’s assumption=reality is work is reduced each S cycle)

$$Damage=\frac{n_1W(S_1)+n_2W(S_2)+\dots}{W_{Failure}}=\frac{n_1W(S_1)}{W_{Failure}}+\frac{n_2W(S_2)}{W_{Failure}}+\dots$$

$$W_{Failure}=N_1W_1(S_1)=N_2W_2(S_2)=N_3W_3(S_3)=\dots$$

$$Damage=\frac{n_1}{N_1}\frac{W(S_1)}{W(S_1)}+\frac{n_2}{N_2}\frac{W(S_2)}{W(S_2)}+\frac{n_3}{N_3}\frac{W(S_3)}{W(S_3)}+\dots=\frac{n_1}{N_1}+\frac{n_2}{N_2}+\frac{n_3}{N_3}+\dots=\sum_i\frac{n_i}{N_i}$$

Example: Miner's Rule

- Then Miner's rule can be modified as
- $Ni = AF(1, i)\, N_1$

$$\text{Effective Damage} \approx \frac{n_1}{N_1} + \frac{n_2}{AF(1,2)N_1} + \frac{n_3}{AF(1,3)N_1} + \bullet\bullet\bullet = \sum_{i=1}^{k} \frac{n_i}{AF(1,i)N_1}$$

Non Equilibrium Thermodynamics, Example 9

- Miner’s Rule for Secondary Batteries

$$Effective \quad Damage \approx \sum_{i=1}^{k} \frac{n_i}{N_i}$$

- Miner’s rule using the n cyclic sum over the Depth of Discharge % (DoD%) i_{th} level stress for battery life pertaining to a certain failure (permanent) voltage drop (such as 10%) of the initially rated battery voltage and then the effective damage done in n_i DoDs% can be assessed when N_i is known

for the i_{th} DoD level.

Thermally Activated Time-dependent (TAT) device degradation models

- Arrhenius Aging Due to Small Parametric Change (due to a changes in the free energy)

$$\frac{da}{dt} = \nu \quad \exp\left(-\frac{\phi(a)}{K_B T} \right) \qquad \phi(a) = \phi(0) + a y_1 + \frac{a^2}{2} y_2 + \ldots$$

where y_1 and y_2 are given by $$y_1 = \frac{\partial \phi(0)}{\partial a} \quad and \quad y_2 = \frac{\partial^2 \phi(0)}{\partial a^2}$$

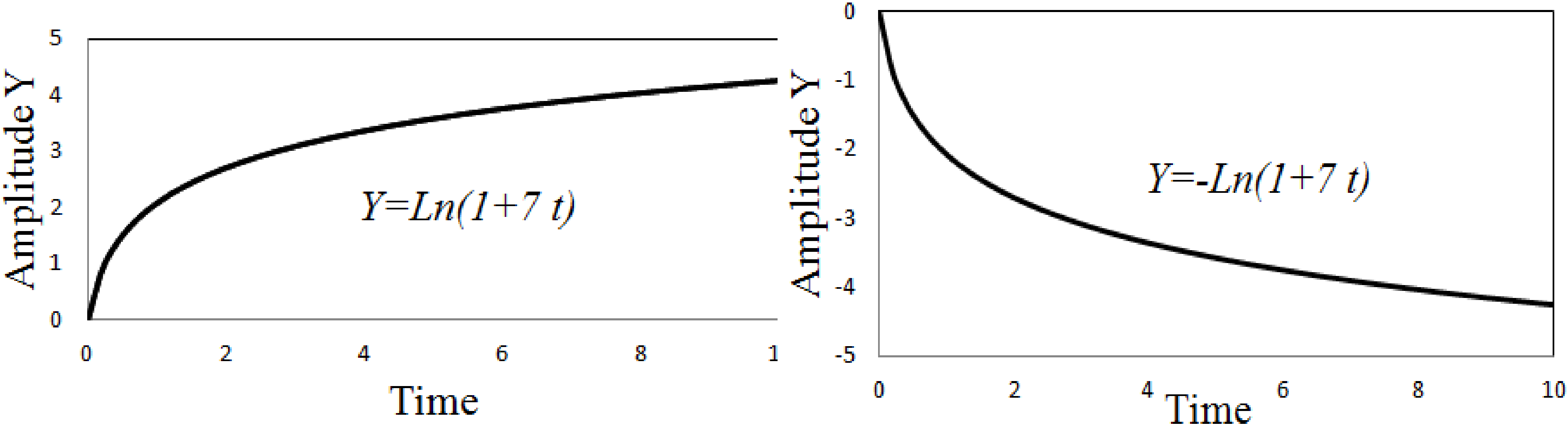
For small parametric change we have

$$\frac{da}{dt} = \nu(T) \quad \exp\left(-\frac{ay1}{K_B T} \right) \qquad \nu(T) = \nu_o \exp\left(-\frac{\phi(0)}{K_B T} \right)$$

Solving

$$a = \frac{\Delta P}{P} \cong A\ \ln[1 + B\,t]$$

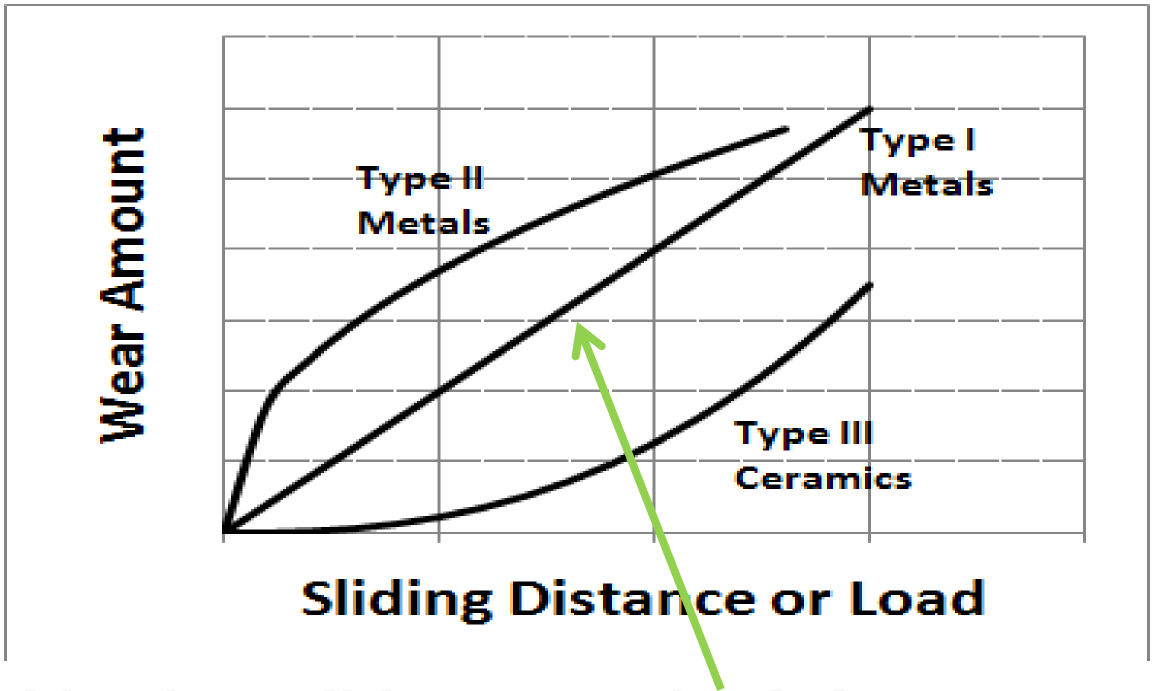
$$A = \frac{K_B T}{y_1} \quad and \quad B = \frac{\nu(T)\,y_1}{K_B T}$$



Examples of Ln(1+B time) aging law with (a) similar to primary and secondary creep stages and (b) similar to primary battery voltage loss. Other key examples include Type II wear, transistor aging.

Wear Modeling

- Common wear types



Type I wear model is covered by the well known Archards linear Wear Model. When logarithmic-in-time aging occurs as is illustrated in Type II wear shown in the Figure (often observed in metals. Here we apply the TAT model. This is characterized by an initially high wear rate then, a steady state low wear rate. Type I shows the case of steady wear in time, Type III typically observed in lapping and polishing for surface finishing of ceramics.

Example 10 : Wear TAT Modeling for Type II

Mass removal M per unit time for an activated process

$$\frac{dM}{dt} = \gamma(T) = \gamma_o \exp\left(-\frac{\phi(0) + \mu M}{K_B T} \right) = \gamma(T)\exp\left(-\frac{\mu\ M}{K_B T} \right)$$

μ as the *activation chemical potential per unit mass*, ϕ is the activation energy for the process and γ is the wear amplitude described in the book chapter.

Model Results

$$M = A \ln(1+Bt) \qquad A = \frac{K_B T}{\mu} \;\; and \;\; B = \frac{\gamma(T)\mu}{K_B T}$$

Note the logarithmic-in-time dependence in the activation wear case differs from the Archard's linear dependence (i.e. $l=vt$). Here we find that when Bt is less than or of the order of 1, the removal amount is large at first then is less as time accumulates - a non linear in time removal. However when $Bt>>1$, the removal is in $\ln(t)$ dependence. Also since $\ln(1+X)\sim X$ for $X<<1$, then this can be approximated as $M \approx ABt = g(T)t$ for $Bt<<1$, which upon substitution agrees with the Archard's wear equation.

Other TAT Model Results Described in the Book Reference

- Ex. 11: TAT Transistor Aging Model
  - Beta degradation of transistors

$$\Delta\beta(t) \cong A \ln[1 + B\,t]$$

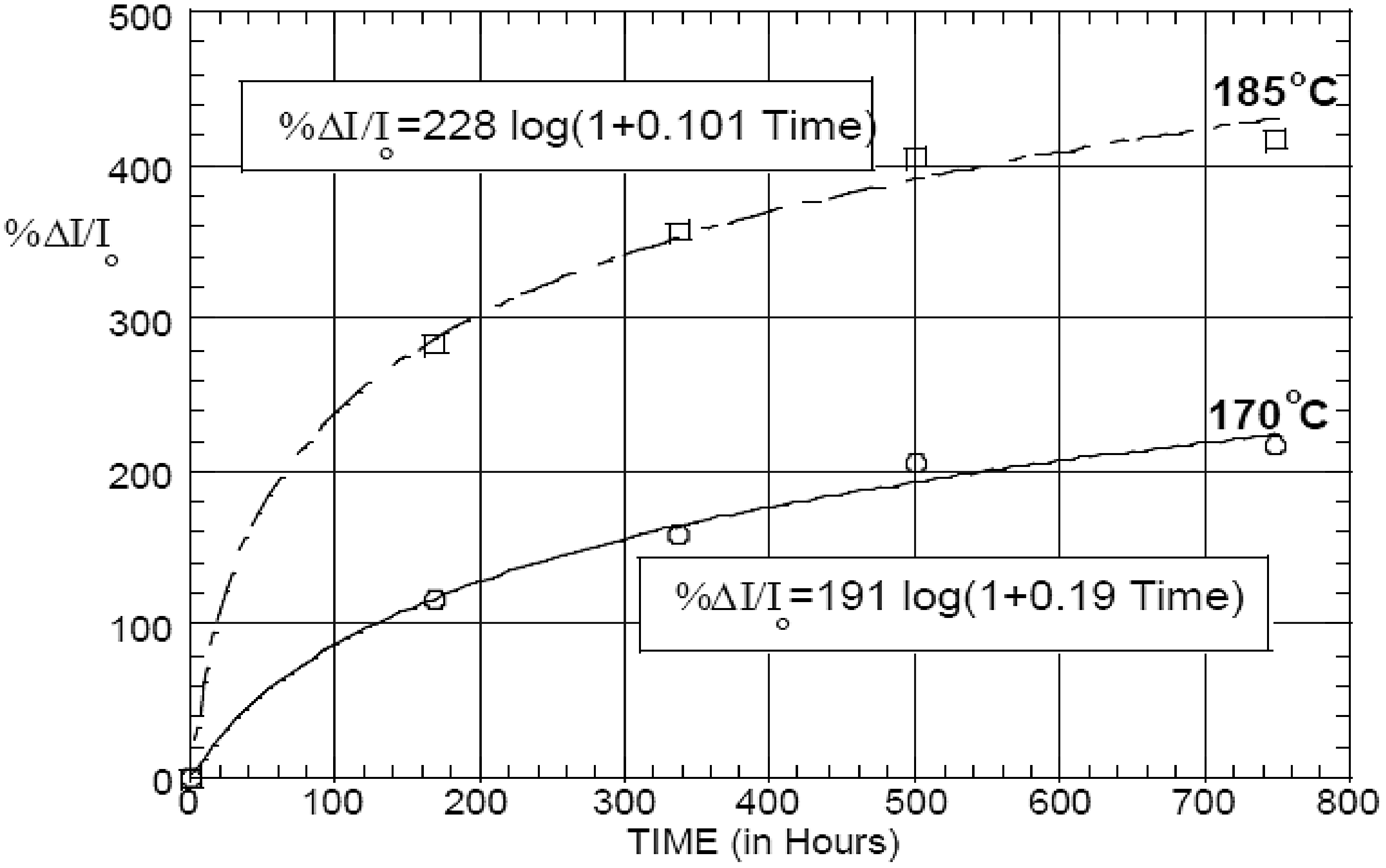
  - MESFET Gate Leakage I $_{\text{Gate-Source}}$ Model

$$\frac{\Delta I_{GS}(t)}{I_{GS}} \cong A \ln[1 + B\,t]$$

- Ex. 12: Creep Model primary & secondary phases in one model

$$\varepsilon = \frac{\Delta L}{L} \cong A \ln[1 + B\,t]$$

FET Model to Data Results



Conclusion

- We presented two methods for finding damage
  - Equilibrium thermodynamic assessment
    - Concept of using entropy as a measure of degradation, how to make such measurements, and the capability to assess damage of complex systems – with an energy approach using entropy damage measurements
  - Non equilibrium thermodynamic assessment
    - Using conjugate work (an energy approach) to assess damage both cyclic and non cyclic over time, an improved method for determining acceleration factors with the work damage approach
- Provide enough information so those interested in this physics of failure approach can decide if they wish to pursue this approach

Appendix Misc. Examples

Selected Results in Non Equilibrium Thermodynamics

- Ex. 13: Corrosion where *I* is the corrosion current

$$Damage\ (corrosion) = \frac{I_1 t_1}{I_2 \tau_2} = AF(1,2)\frac{t_1}{\tau_2}$$

$$Damage\ (corrosion) = 1 = \frac{I_1 \tau_1}{I_2 \tau_2},\ \text{then}\ AF = \frac{\tau_2}{\tau_1} = \frac{I_1}{I_2} = \exp\left\{-\frac{\Delta\varepsilon}{R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right\}\right.$$

Note *I* can optionally be defined in a more sophisticated way

- Ex. 14: In battery corrosion

$$AF = \frac{\tau_2}{\tau_1} = \frac{C_{p2}}{C_{p1}}\left(\frac{I_1}{I_2}\right)^Y$$

Where C_p is the battery capacity, τ is the failure time, I is the corrosion current at a one-ampere discharge rate
per Peukert's Law

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