A Science-Based Theory of Reliability Founded on Thermodynamic Entropy

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 Abstract: Failure data-driven stochastic and probabilistic techniques that underlie reliability analysis of components and structures remain unchanged for decades. The present study relies on a science-based explanation of damage as the source of material failure, and develops an alternative approach to reliability assessment based on the second law of thermodynamics. The common definition of damage, which is widely used to measure the reliability over time, is somewhat abstract, and varies at different geometric scales and when the observable field variables describing the damage change. For example, fatigue damage in metals has been described in several ways including reduction of elasticity modules, variation of hardness, cumulative number of cycle ratio, reduction of load carrying capacity, crack length and energy dissipation. These descriptions are typically based on observable changes in the physical or spatial properties, and exclude unobservable and highly localized damages. Therefore, the definition and measurement of damage is subjective and dependent on the choice of observable variables. However, all damage mechanisms share a common feature at a far deeper level, namely *energy dissipation*. Dissipation is a fundamental measure for irreversibility that, in a thermodynamic treatment of non-equilibrium processes, is quantified by *entropy generation*. Using a theorem relating entropy generation to energy dissipation via generalized thermodynamic forces and thermodynamic fluxes, this paper presents a model that formally describes the resulting damage. This model also contains cases where there is a synergy between different irreversible fluxes, such as in corrosion-fatigue damage where the mechanical deformation rate leading to fatigue is coupled with the electrochemical reaction rate leading to corrosion. Employing thermodynamic forces and fluxes to model the damage process, not only enables us to express the entropy generation in terms of physically measurable quantities including stress diffusion and electrochemical affinities, but also provides a powerful technique for studying the complex synergic effect of multiple irreversible processes. Having developed the proposed damage model over time, one could determine the time that damage accumulates to a level where the component or structure can no longer endure and fails. Existence of any uncertainties about the parameters and independent variables in this thermodynamic-based damage model leads to a time-to-failure distribution. Accordingly, such a distribution can be derived from the thermodynamic laws rather than estimated from the observed failure histories.

1   Introduction

The definition of damage due to the physical mechanisms varies at different geometric and scales. For example, the definition of fatigue damage can vary from nano-scale through the macro-scale. At the atomic level the grain boundary is a likely location where atoms are more loosely packed. At the micro-scale damage is the accumulation of micro-stresses in the neighborhood of cracks. At the meso-scale level, damage might be defined as growth and coalescence of micro-cracks to meso-cracks. However, measuring damage is subject to the physically measurable variables (i.e., observable marker) when dealing with specific failure mechanisms. That means damage in this context is a characterization of the observable symptoms in the form of measurable field variables such as crack length, amount of wear, and degree of deformation (Singpurwalla, 2010). In fact, Arson (2012) states that damage prediction relies on the field variables chosen to describe the anticipated degradation or aging. Singpurwalla (2010) refers to these subjective choices of observable field variables as "observable markers." For example, in the

corrosion-fatigue mechanism material weight loss, change of impedance, density of pits, accumulated number of cycles-to-failure, and crack length may be used as "observable markers" that measure the damage. Therefore, defining a consistent and broad definition of damage is necessary and plausible. To reach this goal, we elaborate on the concept of material damage within the thermodynamic framework.

Thermodynamically, all forms of damage share a common characteristic, which is the dissipation of energy. In thermodynamics, dissipation of energy is the basic measure of irreversibility, which is the main feature of the degradation processes in materials [1]. Chemical reactions, release of heat, diffusion of materials, plastic deformation, and other means of energy production involve dissipative processes. In turn, dissipation of energy can be quantified by the *entropy generation* within the context of irreversible thermodynamics. Therefore, dissipation (or equivalently entropy generation) can be considered as a substitute for characterization of damage.

The common practice in damage analysis and prediction of structural life and integrity is through the application of the traditional reliability and Physics-of-Failure (PoF) methods. The traditional generic handbook-based reliability prediction methods such as those advocated in MIL-HDBK-217F [2], Telcordia SR-332 [3], and FIDES [4] rely on analysis of the field data (with incoherent operating and environmental conditions), with the assumption of the constant failure rates. Numerous studies have shown that misleading and inaccurate results from applications of these handbooks can lead to poor designs, incorrect reliability prediction and operating decisions [5, 6, 19, 20]. The PoF models such as the Coffin-Manson model [5], Norris-Landzberg model [6] and Bayerer's model [7] offer more rigorous and improved reliability estimation approach. However, these empirically-based methods are limited to simple failure mechanisms and are hard to model multiple competing and common cause failure mechanisms.

In contrast, with the empirically-based PoF approach to reliability prediction, which considers only the most predominant failure mechanisms ([8, 9]), the definition of damage in the context of the thermodynamic entropy allows for the incorporation of all underlying dissipative processes. For example in the case of corrosion-fatigue, consider the physically measurable quantities such as stress and electrochemical affinity of the oxidation-reduction electrode reaction ($Me \Leftrightarrow Me^{z+} + ze$) of a metal. The entropy as a state function is independent of the path of the failure (which commonly depends on factors such as geometry, load, frequency of load, etc.) from the initial state to the final failed state of the material, considering a known failure threshold (endurance limit) [10]. Entropy provides a science-based approach to model a wide range of damage processes with favorable results in fracture mechanics, fatigue damage analysis [10, 11] and tribological processes such as friction and wear [12, 13]. Additionally, it provides a powerful technique for studying the synergistic effects arising from interaction of multiple processes [18].

However, lack of detailed knowledge about the independent variables that generate entropy such as the exact loading conditions applied to a structure, materials-to-materials variability, environmental and seasonal factors means there would be uncertainties about the entropic-based trajectory of cumulative damage. While in the absence of such uncertainties an exact time of failure can be calculated, existence of such uncertainties will lead to estimation of a time-to-failure distribution.

The remainder of this paper is organized as follows. Section 2 presents the features of material damage. Section 3 describes our construction of the entropy model. Section 4 describes the relationship between the damage and entropy generation. Section 5 links the entropy, as an index of damage, to the reliability assessment and section 6 offers concluding remarks.

2   A Characterization of Material Damage

Damage can be viewed as surface or volumetric deterioration of materials. For example, fatigue and creep are processes that cause volumetric damage in structures, while corrosion and wear cause surface damage. At the macroscopic level, realization of material damage becomes difficult and significantly dependent on

the type of volumetric or surface damage. Lemaitre and Chaboche [14] state that unless any macroscopic discontinuity or permanent distortion can be observed, it would be very difficult to assess integrity and health of structural materials. The common practice of damage evaluation is through the quantification of the symptoms or observable markers of damage (e.g., crack size, density of crack, depth of the pit, weight loss) and other mechanical markers (e.g., reduction of the elastic modulus, accumulation of plastic strain, or change in viscoplastic properties). Difficulties to develop a consistent definition of damage from physical and mechanical points of view have compelled researchers to look for a microscopically consistent definition in the context of the continuum damage mechanics [14]. For example, in the continuum damage mechanics the damage, D, as an internal variable is defined as the effective surface density of microdefects:

$$D = \frac{S_D}{S} \tag{1}$$

where S_D is the damage surface area and S is the initial cross section area. Due to the difficulty in direct measurement of the density of defects on the surface or volume of materials, Lemaitre [15] used the strain equivalent principle to correlate between other measurable properties of material (e.g. variation of elastic strain, module of elasticity, micro-hardness, density, and plastic strain) and damage. However, these different damage indexes do not provide a consistent measure of damage, including all the observable and unobservable damages.

At the micro-level, however, material damage can be defined in a more coherent way. In fact, at the nano-scale, damage may refer to breaking and reestablishment of the interatomic bonds in crystalline metals and polymers ([16]). Based on this fundamental definition of damage, meso-scale characteristics of damage such as dislocations, slips, micro-cavities, and micro-cracks can be quantified.

As discussed above, several definitions and measures of damage exist, however, the concept of damage is somewhat abstract, and definitions are relative. All damage mechanisms share a common characteristic at a much deeper level, i.e., the "dissipation" of energy. Dissipation can be described well within the context of non-equilibrium thermodynamics using the second law of thermodynamics. In a thermodynamics treatment of non-equilibrium irreversible processes, dissipation is quantified by the "entropy generation". We consider this characterization of damage highly general, consistent and scalable. In the following section the focus is on the formulation of the entropy generation caused by dissipative mechanisms, using the corrosion-fatigue as a demonstration example.

3   Total Entropy Produced in a System
Consistent with the second law of thermodynamics, entropy does not obey a conservation law. Therefore, it is essential to relate the entropy not only to the entropy crossing the boundary between the system and its surroundings, but also to the entropy produced by the processes taking place inside the system. Processes occurring inside the system may be reversible or irreversible. Reversible processes inside a system may lead to the transfer of the entropy from one part of the system to other part of the interior, but do not generate entropy. Irreversible processes inside a system, however, result in generation of the entropy, and hence in computing the entropy they must be taken into account.

Using the second law of thermodynamic, it is possible to express the variation of total entropy flow per unit volume, $dS,$ in the form of

$$dS = d^r S + d^d S \tag{2}$$

where $d^r S$ is the entropy supplied to the system by its surroundings through transfer of matters and heat (e.g., in an open system where wear and corrosion mechanisms occur). The rate of exchanged entropy is obtained as

$$\frac{d^r S}{dt} = -\int^\Omega J_s \cdot n_s dA \tag{3}$$

where J_s is a vector of the total entropy flow per unit area , crossing the boundary between the system and its surroundings, and n_s is a normal vector. Similarly, $d^d S$ is the entropy produced inside of the system, which can be obtained from Eq. 4,

$$\frac{d^d S}{dt} = \int^V \sigma dV \tag{4}$$

where, σ is the entropy generation per unit volume per unit time. The second law of thermodynamics states that $d^d S$ must be zero for reversible transformations and positive ($d^d S > 0$) for irreversible transformations of the system.

The balance equation for entropy shown in Eq. 5 can be derived using the conservation of energy and balance equation for the mass.

$$\frac{dS}{dt} + \nabla J_s = \sigma \tag{5}$$

This gives us an explicit expression for total entropy in terms of reversible and irreversible processes [14, 17, 18]

$$\frac{dS}{dt} = -\nabla \cdot \left(\frac{J_q - \Sigma \mu_k J_k}{T} \right) - \frac{1}{T^2} J_q \cdot \nabla T - \Sigma_{k=1}^n J_k \left(\nabla \frac{\mu_k}{T} \right) - \frac{1}{T} \Sigma_{f=1}^n F_k J_f - \frac{1}{T} \Pi : \nabla V - \frac{1}{T} \Sigma_{j=1}^r v_j A_j \tag{6}$$

where, T is the temperature, μ_k the chemical potential, J_q the heat flux, J_k the diffusion flow, v_i the chemical reaction rate, Π the stress tensor, ∇V the velocity gradient (equal to strain rate $\dot{\epsilon}$), $A_j = -\Sigma_k \mu_k v_{jk}$ the chemical affinity or chemical reaction potential difference, F_k the force due to external field, and J_f the corresponding flux. Each term in Eq. 6 is derived from various mechanisms involved, which define the macroscopic state of the complete system. External forces may be resulted from different factors including electrical field, magnetic field, gravity field, etc., where the corresponding fluxes are electrical current, magnetic current and velocity.

By comparing Eq. 6 with Eq. 5 we can make the identifications

$$J_s = \frac{J_q - \Sigma \mu_k J_k}{T} \tag{7}$$

$$\sigma = -\frac{1}{T^2} J_q \cdot \nabla T - \Sigma_{k=1}^n J_k \left(\nabla \frac{\mu_k}{T} \right) - \frac{1}{T} \Sigma_{f=1}^n F_k J_f - \frac{1}{T} \Pi : \nabla V - \frac{1}{T} \Sigma_{j=1}^r v_j A_j \tag{8}$$

where, Eq. 7 shows the entropy flux resulted from heat and material exchange. Equation 8 represents the total energy dissipation terms from the system that from left to the right include heat conduction energy, diffusion energy, external force energy, mechanical energy, and chemical energy. Equation 8 is fundamental to non-equilibrium thermodynamics, and represents the entropy generation σ as the bilinear form of forces and fluxes as

$$\sigma = \Sigma_{i=1}^m X_i J_i \tag{9}$$

It is through this form that the contribution from the applicable thermodynamic forces and fluxes are expressed. For example, in the case of a chemically reactive system, the chemical affinity A_j drive the

chemical reaction with velocities v_j, the mechanical stress cause the deformation rate, the concentration gradient cause the diffusion rate, and the temperature gradient generate the heat flow.

In the linear non-equilibrium thermodynamics (LNT) theory whereby the variation of thermodynamic forces and fluxes are small, the components of the thermodynamic fluxes, J_i, are assumed to be a linear combination of the components of the thermodynamic forces, X_i, so that [19]

$$J_i = \sum_{k=1}^{n} L_{ik} X_k \tag{10}$$

where, L_{ik}'s are the phenomenological coefficients. According to the Onsager reciprocity theorem [19], the equation of motion for each individual particle is time reversible as in classical dynamics or quantum mechanics. The macroscopic result obtained from this assumption is that $L_{ik} = L_{ki}$. It is worth to note that, the LNT application is limited to linear systems with no general means of minimizing entropy generation, which is implied by Prigogine's theorem[1] as a special case of Zeigler principle [20]. Further, the phenomenological coefficients of LNT must be determined experimentally. An advantage is that it can relate the fluxes and their coupling in a very fast process by using a linear relationship [21, 22]. The Seebeck effect, Furiers's law of heat conduction, Fick's law of diffusion, Ohm's law of electrical condition, and the Navier-Stokes equations for fluids may be formally derived from the LNT [17].

For example, damage in the corrosion-fatigue damage mechanism is produced by the synergy between two irreversible fluxes of anodic dissolution current density and the plastic deformation [23]. Gutman [23] first identified the influence of plastic deformation on anodic dissolution rate and vice versa (i.e., the mechanochemical effect), where the entropy generation is the summation of entropy generation due to electrochemical reaction and plastic deformation. Summing the contributions of the mechanical and electrochemical processes, we can write the total entropy generation for combined effect of plastic deformation and anodic and catholic dissolution as:

$$T\sigma = \Pi : \dot{\boldsymbol{\varepsilon}}_{\boldsymbol{P}} + \tilde{A} i_{corr} \tag{11}$$

where $\tilde{A}$ is the electrochemical and mechanochemical potential losses (over-potential). Employing LNT theory, we can write the following system of phenomenological equations to take the cross effects of two processes into consideration

$$\dot{\varepsilon}_P = L_{11}\Pi + L_{12}\tilde{A} \tag{12}$$

$$i_{corr} = L_{21}\Pi + \mathrm{L}_{21}\tilde{A} \tag{13}$$

4   Physical Damage versus Total Entropy Generation

To validate the entropy as an appropriate parameter representing the physical or mechanical damages (e.g. weight loss, crack size, young modulus), Bryant et al. link quantitative and observable markers of degradation processes leading to damage (e.g. wear volume, crack size and corrosion mass loss) to the associated entropy generation [24]. They derived the damage rate $\dot{w} = \Sigma_i \dot{w}_i = \Sigma_i \Sigma_j Y_i^j J_i^j$ as a linear combination of the components of entropy generation σ_i produced by the dissipative processes.

$$\dot{w} = \Sigma_i B_i \sigma_i \tag{14}$$

where, B_i represents the degradation coefficient that relates the generalized degradation force, Y_i, to generalized thermodynamic force, X_i, so that $Y_i = B_i X_i$. In an application of this approach, they also show

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[1] According to this theory the entropy production given in Eq. 9 takes a minimum on stationary states.

that in wear, the rate of weight loss derived from the concept of entropy generation is in agreement with Archard's sliding wear model [25], and Doelling et al. experimental results[26]. Amiri et al. showed a linear relationship between the dissipative energy and wear volume [12]. Ontiveros et al., denoted a linear correlation between the cumulative plastic strain energy and cycles-to-crack initiation in high-cycle fatigue of Aluminum alloys [11].

5   Reliability Assessment Using Entropy as an Index of Damage

It was stated earlier that damage caused through a degradation process could be viewed as the consequence of dissipation of energy that can be measured and expressed by entropy such that:

$$Damage \equiv Entropy$$

In the earlier discussion in this paper it was shown (through Eq. 5) that one could express the total entropy per unit time per unit volume for the individual dissipation processes resulting from the corresponding failure mechanisms. Therefore, the evolution trend of the damage, D, is obtained from

$$D|t \sim \int_0^t [\dot{S}|X_i(u), J_i(u)]du \tag{15}$$

where $D|t$ is the monotonically increasing cumulative damage starting at time t from a theoretically zero value or practically some initial damage value. When D reaches a predefined (often subjective) level of endurance it may be assumed beyond that point the component or structure fails. It is worth to note that failure in this context is the point when an item becomes effectively nonfunctional (but possibly still operational). That is failure is considered as the point where the item is no longer meeting a functionality requirement (e.g., an acceptable performance level or an endurance limit such as a given level of thermodynamic efficiency).

Because entropy as a parameter of degradation includes all observable damage markers (cracks, wear debris and pit densities) and unobservable damages such as subsurface dislocations, slip and micro-cavities, definition of a single failure threshold might not be possible due to long stretch of damage measurement from nono-scale to macroscopic scale. In this case, the cumulative damage and alternatively entropy endurance level can be estimated through the measurement of certain observable damage markers. The correlation between the observable damage markers and entropy, justified by several studies [10, 11, 12], enables the definition of failure threshold on the basis of observable markers. In the other word, the damages grow, coalesce and eventually the weakest link among all coalesces damages manifests itself as an observable damage which causes failure.

Materials, environmental, operational and other variability in degradation forces impose uncertainties on the cumulative damage, D. Existence of such uncertainties leads to confidence intervals around the mean value and about the time that a failure occurs (as depicted in Figure 1). This figure shows how the interfaces of the accumulated damage and endurance level result in the probability density function (PDF) of the time-to-failures, which is the variable of interest in most reliability analysis. It is self-evident that the probability that the random variable, $D|t$, (i.e., the cumulative damage at time, t) exceeds the constant endurance level, D_f (thus causing the failure), must be equal to the probability that the random variable time-to-failure is less than t. Accordingly, the magnified section in Figure 1 depicts the cumulative probability of damage as the diagonal shaded area, and the cumulative time to failure probability as the solid shaded area.

 Accordingly, assuming the constant endurance limit, D_f, one can derive the time-to-failure distribution, $g(t)$, from the thermodynamically-based damage relation expressed by Eq. 15,

$$\int_0^t g(x)dx = \int_{D_f}^{\infty} f(D|t)dD) \tag{16}$$

where $f(D|t)$ is the PDF of the damage at time t. The corresponding time to failure PDF, $g(t)$, would be

$$g(t) = \frac{d}{dt}\int_{D_f}^{\infty} f(D|t)dD \tag{17}$$

Obviously, the reliability function can be expressed as

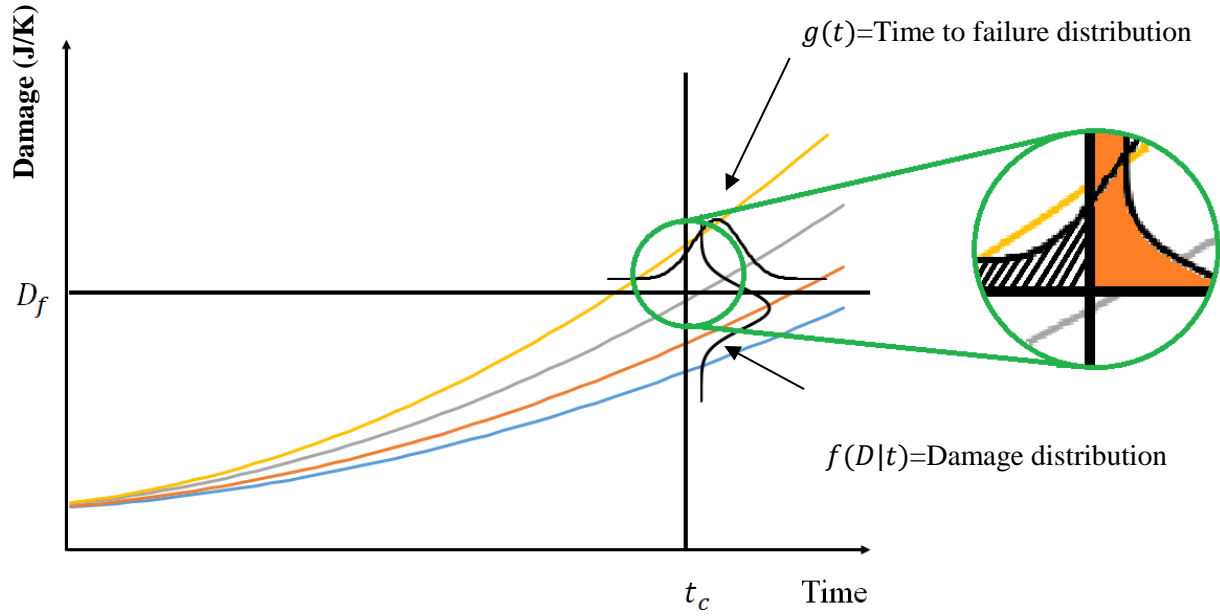$$R(t) = \int_t^{\infty} g(t)dt = 1 - \int_{D_f}^{\infty} f(D|t)dD \tag{18}$$

Figure 1: Damage- endurance modeling.

Similar to the uncertainties about the amount of damage, the endurance limit, D_f, may also be uncertain because composition of materials and thus their strengths varies from sample to sample. In this case, a failure occurs when the damage in a component exceeds its endurance level. The probability that no failure occurs is equal to the probability that the random variable, D, is less than the random variable, D_f, describing the component endurance level.

$$R(t) = \Pr(D|t < D_f|t) \tag{19}$$

Where $R(t)$ is the relaibilty of component at time t. Knowing the PDFs of the random variables D and D_f expressed by $f(D)$ and $h(D_f|t)$, the PDF of the time-to-failure distribution can be obtained by

$$R(t) = 1 - \int_0^{\infty} h(D_f|t)dD_f \int_{D_f}^{\infty} f(D|t)dD, \tag{20}$$

and

$$g(t) = -\frac{d}{dt}R(t) \tag{21}$$

It is possible that the PDF of the endurance limit is independent of time (i.e., $D_f|t \approx D_f$). If multiple dissipative forces are at work then using the weakest link principle

$$R(t) = \prod_{i=0}^{n}\left\{1 - \int_0^\infty h(D_{f_i}|t)dD_{f_i}\int_{D_{f_i}}^\infty f(D_i|t)dD_i\right\} \tag{22}$$

Again Eq. (20) serves as the basis to derive the PDF of the time-to-failure.

6   Conclusions

This paper presents a thermodynamic framework for the degradation level assessment using entropy generation as a measure of damage. It suggests that a unified measure of damage can be defined based on the entropy generation concept. Applying the entropic method can improve our understanding of the degradation mechanism and the quantification of damage. Entropy, as a state function, is independent of the failure path, and provides a formal means to analyze the synergy between different degradation mechanisms and forces. The general entropy generation function is derived in terms of energy losses due to heat conduction, diffusion losses, mechanical dissipations, chemical losses and external force field effects (e.g. magnetic, electrical and gravity fields). It is shown that entropy generation and damage are related. However, the entropy generation function is subject to various stochastic variations of forces that cause damage. The reliability model is built off of the relationship between damage PDF, endurance limit distribution and time-to-failure PDF.

This paper discusses a fundamental foundation for a science-based explanation of damage as a source of material failure and thus materials reliability. As such we offer an alternative approach for reliability assessment based on the second law of thermodynamics. As the next step, which is validating the proposed framework, we are now studying the entropy growth rate as a degradation parameter for the corrosion-fatigue mechanism in materials. This approach could open the window for further exploration of the applications of thermodynamics for reliability assessment and analysis of materials and prognosis and health management of critical components and structures.

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