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An Irreversible Thermodynamics Theory for Damage Mechanics of Solids

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ABSTRACT: The entropy production is a non-negative quantity based on irreversible thermodynamics and thus serves as a basis for the systematic description of the irreversible processes occurring in a solid. In this paper, a thermodynamic framework has been presented for damage mechanics of solid materials, where entropy production is used as the sole measure of damage evolution in the system. As a result, there is no need for physically meaningless empirical parameters to define a phenomenological damage potential surface or a Weibull function to trace damage evolution in solid continuum. In order to validate the model, predictions are compared with experimental results, which indicates that entropy production can be used as a damage evolution metric. The theory is founded on the basic premise that a solid continuum obeys the first and the second laws of thermodynamics.

KEY WORDS: conservation laws, irreversible thermodynamics, damage mechanics, entropy production, thermo-mechanical coupling.

INTRODUCTION

THE SCIENCE OF thermodynamics, which began by treating the relations among heat, work and the properties of the systems in equilibrium, has developed into a very general science of energetics for all types of systems: mechanical, chemical or electrical, whether in equilibrium or not (Yourgrau et al., 1966; Haase, 1968; Germain et al., 1983; Ericksen, 1998). Irreversible thermodynamics provides a general framework for the macroscopic description of irreversible processes. In irreversible thermodynamics, the so-called balance equation for the entropy plays a central role. The equation expresses the fact that the entropy of a volume element changes with time

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for two reasons. First, it changes because entropy flows into the volume element. Second, it changes because there is an entropy source due to irreversible phenomena inside the volume element. The entropy source is always a non-negative quantity, since entropy can only be created, never destroyed. For reversible processes the entropy source vanishes.

To relate the entropy source explicitly to the various irreversible processes that occur in a solid system, one needs the macroscopic conservation laws of mass, momentum and energy in local, i.e. differential form. These conservation laws contain a number of quantities such as the diffusion flow, the heat flow and the stress tensor, which are related to the transport of mass, energy and momentum. The entropy source may then be calculated by using the thermodynamics Gibbs relation, which connects the rate of the change in entropy in the medium to the rate of the change in energy and work. "It turns out that the entropy source has a very simple appearance: it is a sum of terms each being a product of a flux characterizing an irreversible process, and a quantity called thermodynamic force, which is related to the non-uniformity of the system..."(Groot and Mazur, 1962). The entropy source strength can thus serve as a basis for the systematic description of the irreversible processes occurring in a solid system.

Yet the entropy balance equation and laws of conservation cannot alone be used to solve the initial and boundary value problem, since this set of equations contain the irreversible flux as unknown parameter. These equations must be tied to the system specific (in this case solid continuum) relationships to be meaningful and facilitate the solution of initial or boundary value problems.

CONSERVATION LAWS

Thermodynamics is based on two fundamental laws: the first law of thermodynamics or law of conservation of energy, and the second law of thermodynamics, or entropy law. A systematic macroscopic scheme for the description of irreversible processes must also be built upon these two laws. However, it is necessary to formulate these laws in a way suitable for the purpose at hand. Since we wish to develop a theory applicable to systems of which the properties are continuous functions of space coordinates and time, we shall give a local formulation of the law of thermodynamics. As the local momentum and mass densities may change in time, we shall also need local formulations of the laws of conservation of momentum and mass. Here, the thermodynamic system is assumed to be a collection of continuous matter. The system is not an interchanging matter with its surroundings; the bounding surface of the system moves with the flow of matter.

Conservation of Mass

The total mass is conserved, i.e. that the total mass in any volume element of the system can only change if matter flows into (or out of) the volume element, which can be expressed as

$$\frac{\partial \rho}{\partial t} = -\mathrm{div} \rho \upsilon \tag{1}$$

where ρ is the density, υ is the velocity. This equation has the form of a so-called balanced equation: the local change of the density is equal to the negative divergence of the flow of mass.

Momentum Principle

Consider a given mass of the medium acted upon by external surface **t** and body force **b**, then the momentum principle can be expressed as (Malvern, 1969):

$$\rho \frac{d(1/2)\boldsymbol{\upsilon}^2}{dt} = \mathrm{div}(\boldsymbol{\sigma} \cdot \boldsymbol{\upsilon}) - \boldsymbol{\sigma} : \mathrm{Grad}\ \boldsymbol{\upsilon} + \rho \mathbf{b} \cdot \boldsymbol{\upsilon} \tag{2}$$

where $\boldsymbol{\sigma}$ is the symmetric stress tensor for nonpolar case. Grad $\boldsymbol{\upsilon}$ can be written as the sum of a symmetric rate of deformation tensor **D** and a skew symmetric spin tensor **W**:

$$\mathrm{Grad}\ \boldsymbol{\upsilon} = \mathbf{D} + \mathbf{W} \tag{3}$$

With the help of Equations (1) and (3), Equation (2) becomes:

$$\frac{\partial (1/2)\rho \boldsymbol{\upsilon}^2}{\partial t} = -\mathrm{div}\left(\frac{1}{2}\rho \boldsymbol{\upsilon}^2 \cdot \boldsymbol{\upsilon} - \boldsymbol{\sigma} \cdot \boldsymbol{\upsilon}\right) - \boldsymbol{\sigma} : \mathbf{D} + \rho \mathbf{b} \cdot \boldsymbol{\upsilon} \tag{4}$$

Considering conservative forces which can be derived from a potential ψ independent of time (Groot and Mazur, 1962):

$$\mathbf{b} = -\mathrm{grad}\ \psi, \quad \frac{\partial \psi}{\partial t} = 0 \tag{5}$$

we establish an equation for the rate of change of the potential energy density $\rho\psi$:

$$\frac{\partial\rho\psi}{\partial t} = -\text{div } \rho\psi\boldsymbol{v} - \rho\mathbf{b}\cdot\boldsymbol{v} \tag{6}$$

Adding Equations (4) and (6), we obtain the rate of change for the sum of the kinetic energy $(1/2)\rho\boldsymbol{v}^2$ and the potential energy $\rho\psi$:

$$\frac{\partial\rho((1/2)\boldsymbol{v}^2 + \psi)}{\partial t} = -\text{div } \{\rho\left(\frac{1}{2}\boldsymbol{v}^2 + \psi\right)\cdot\boldsymbol{v} - \boldsymbol{\sigma}\cdot\boldsymbol{v}\} - \boldsymbol{\sigma} : \mathbf{D} \tag{7}$$

Conservation of Energy

Suppose that the only energy transfer to the system is by mechanical work done on the system by surface tractions and body forces, by heat exchange through the boundary, and possibly by distributed internal heat sources. According to the principle of conservation of energy, the total energy content within an arbitrary volume in the system can only change if energy flows into (out of) the volume considered through its boundary, which can be expressed as:

$$\frac{\partial\rho e}{\partial t} = -\text{div } \mathbf{J_e} + \rho r \tag{8}$$

where r is the distributed internal heat source per unit mass, e is the total specific energy per unit mass including the specific kinetic energy $(1/2)\boldsymbol{v}^2$, the specific potential energy ψ and the specific internal energy u (Groot and Mazur, 1962):

$$e = \frac{1}{2}\boldsymbol{v}^2 + \psi + u \tag{9}$$

and $\mathbf{J_e}$ is the total energy flux per unit surface and unit time including a convective term $\rho e\boldsymbol{v}$, an energy flux $\boldsymbol{\sigma}\cdot\boldsymbol{v}$ due to the mechanical work performed on the system, and finally a heat flux $\mathbf{J}_q$ (Groot and Mazur, 1962):

$$\mathbf{J}_e = \rho e\boldsymbol{v} - \boldsymbol{\sigma}\cdot\boldsymbol{v} + \mathbf{J}_q \tag{10}$$

Subtracting Equation (7) from Equation (8), we obtain, using Equation (1), (9) and (10), the balance equation for the specific internal energy u:

$$\rho\frac{du}{dt} = -\text{div } \mathbf{J}_q + \boldsymbol{\sigma} : \mathbf{D} + \rho r \tag{11}$$

ENTROPY BALANCE

Thermodynamics in traditional sense is concerned with the study of reversible transformation. For an irreversible process in which the thermodynamic state of a solid changes from some initial state to a current state, it is assumed that such a process can occur along an imaginary reversible isothermal path, which consists of a two-step sequence (Krajcinovic, 1996). This is the so-called local equilibrium assumption, which postulates that the thermodynamic state of a material at a given point and instant is completely defined by the knowledge of the values of a certain number of variables at that instant. The method of local state implies that the laws that are valid for a macroscopic system remain valid for infinitesimally small parts of it. The processes defined in this way will be thermodynamically admissible if, at any instant of evolution, the Clausius–Duhem inequality is satisfied.

According to the principles of thermodynamics, two more new variables, temperature T and entropy S, are introduced for any macroscopic system. The entropy expresses a variation of energy associated with a variation in the temperature. The entropy of the universe, taken as system plus whatever surroundings are involved in producing the change within the system, can only increase. The variation of the entropy dS may be written as the sum of two, and only two, terms for a closed system:

$$dS = dS_e + dS_i \tag{12}$$

where dS_e is the entropy derived from the transfer of heat from external sources across the boundary of the system, and dS_i is the entropy produced inside the system. The second law of thermodynamics states that dS_i must be zero for any reversible transformation and positive for irreversible transformation of the system, namely:

$$dS_i \geq 0 \tag{13}$$

The entropy supplied, dS_e, on the other hand may be positive, zero or negative, depending on the interaction of the system with its surroundings.

In order to relate dS_i to the various irreversible phenomena occurring inside the system, we rewrite Equations (12) and (13) in local form as:

$$\rho \frac{ds}{dt} = -\text{div}\ \mathbf{J}_S + \gamma \tag{14}$$

$$\gamma \geq 0 \tag{15}$$

where $S = \int^V \rho s dV$, $(dS_e/dt) = -\int^\Omega (\mathbf{J}_S + \rho s \boldsymbol{v}) \cdot d\Omega$, $dS_i/dt = \int^V \gamma dV$, and s is the entropy per unit mass, $\mathbf{J}_S$ is the entropy flux, and γ is the entropy production per unit volume and unit time.

In equilibrium, the total differential of entropy is given by the Gibbs relation that combines the first and second laws. For a closed system, the Gibbs relation can be written as in the form of local variables

$$Tds = du - dw_{\text{ava}} \tag{16}$$

where w_{ava} is the available work, namely the work stored in the system during a process. It should be pointed out that the available work, unlike the irreversible work, is not a function of the process path. It depends only on the end states of the process for a given environmental temperature. The available work is the maximum amount of work that could be produced by a system between any two given states (Li, 1989).

Inserting the Equations (11), for du/dt, into Equation (16), yields:

$$\rho\frac{ds}{dt} = -\text{div}\ \frac{\mathbf{J}_q}{T} - \frac{1}{T^2}\mathbf{J}_q \cdot \text{grad}\ T + \frac{1}{T}\boldsymbol{\sigma} : \mathbf{D} - \frac{\rho}{T}\frac{dw_{\text{ava}}}{dt} + \frac{\rho r}{T} \tag{17}$$

which follows that the expressions for the entropy production are given by:

$$\gamma = \frac{1}{T}\boldsymbol{\sigma} : \mathbf{D} - \frac{\rho}{T}\frac{dw_{\text{ava}}}{dt} - \frac{1}{T^2}\mathbf{J}_q \cdot \text{grad}\ T + \frac{\rho r}{T} \tag{18}$$

Equation (18) represents the entropy production caused by the dissipations. The sum of the first two terms is called the intrinsic dissipation or mechanical dissipation, which consists of plastic dissipation plus the dissipation associated with the evolution of other internal variables. The last two terms are the thermal dissipation due to the conduction of heat and internal heat source. Finally it is noted that Equation (17) satisfies the Clausius–Duhem inequality:

$$\boldsymbol{\sigma} : \mathbf{D} - \rho\left(\frac{d\varphi}{dt} + s\frac{dT}{dt}\right) - \mathbf{J}_q \cdot \frac{\text{grad}\ T}{T} \geq 0 \tag{19}$$

where φ is the specific Helmholtz free energy which is defined as the difference between the specific internal energy density u and the product between the absolute temperature T and specific entropy s:

$$\varphi = u - Ts \tag{20}$$

Since solid opaque bodies are of primary interest here, heat is transferred from point to point within this body solely by conduction. Experimental Fourier's law of heat conduction for isotropic bodies may be stated as follows (Boley and Weiner, 1988):

$$\mathbf{J}_q = -k \text{ grad } T \tag{21}$$

where k, with typical units of $Btu/ft \cdot h \cdot {}^\circ\mathrm{F}$, is termed the thermal conductivity of the solid. Then the expression for the internal entropy source can be simplified as:

$$\gamma = \frac{1}{T}\boldsymbol{\sigma} : \mathbf{D} - \frac{\rho}{T}\frac{dw_{\mathrm{ava}}}{dt} + \frac{k}{T^2}\left|\text{grad } T\right|^2 + \frac{\rho r}{T} \tag{22}$$

FULLY COUPLED THERMO-MECHANICAL EQUATIONS

The coupling of continuum mechanics and thermodynamics requires the selection of a certain number of state variables. We limit ourselves to two observable variables: the temperature T and the total strain ε for elasticity. For dissipative phenomena the current state depends on the history which is represented, in the method of local state, by values of internal variables at each instant. For general study, here these variables will be denoted by $V_k (k = 1,2 \cdots)$ representing either a scalar or a tensorial variable. The relations existing between the energy, stress tensor and strain tensor can be obtained using the formalism of thermodynamics with internal variables. Here we choose the specific Helmholtz free energy φ, which depends on observable variables and internal variables. At small strains, the following expressions can be defined:

$$\boldsymbol{\sigma} = \rho\frac{\partial\varphi}{\partial\varepsilon^e}, \quad s = -\frac{\partial\varphi}{\partial T}, \quad A_k = \rho\frac{\partial\varphi}{\partial V_k}, \tag{23}$$

where A_k is the thermodynamic forces associated with the internal variables V_k. s, $\boldsymbol{\sigma}$ and A_k constitute the associated variables. The vector formed by the variables is the gradient of the function φ in the space of the variables T, ε^e and V_k. Then the fully coupled thermo-mechanical equations can be derived as (Lemaitre and Chaboche, 1990):

$$k\nabla^2 T = \rho C\dot{T} - \boldsymbol{\sigma} : \underline{\varepsilon}^p + A_k V_k - \rho r - T\left(\frac{\partial\boldsymbol{\sigma}}{\partial T} : \underline{\varepsilon}^e + \frac{\partial A_k}{\partial T}\dot{V}_k\right) \tag{24}$$

where ε^p is the inelastic strain, C is the specific heat, and r is the distributed internal heat source per unit mass.

The fully coupled thermo-mechanical equation can simulate the evolution of temperature in the solid due to any mechanical work with properly imposed boundary conditions. $A_k\dot{V}_k$ represents the nonrecoverable energy stored in the materials corresponding to other dissipated phenomena. It represents only 5–10% of the term $\boldsymbol{\sigma} : \underline{\varepsilon}^p$ and is often negligible (Lemaitre and Chaboche, 1990):

$$A_k\dot{V}_k \approx 0 \tag{25}$$

So, we can write the fully coupled elastoplastic thermo-mechanical equation as:

$$k\nabla^2 T = \rho C\dot{T} - \boldsymbol{\sigma} : \underline{\varepsilon}^p - \rho r - T\frac{\partial \boldsymbol{\sigma}}{\partial T} : \underline{\varepsilon}^e \tag{26}$$

which has been used to simulate the thermal effects on the material behavior by many researchers (Sluzalec, 1988; Hong, 1999). Equation (26) also allows us to calculate heat flux $\mathbf{J}_q$ generated due to elastic and/or inelastic work in a solid body.

APPLICATION IN DAMAGE MECHANICS

Changes in the real world are always irreversible processes because of friction, which results in the production of entropy and thus a permanent change in the universe (Dehoff, 1993). Damage is the progressive deterioration which occurs in materials prior to failure. Cumulative damage analysis plays a key role in life prediction of components and structures subjected to load histories. As a result, many damage models have been proposed in the literature, such as linear damage models, nonlinear damage models, linear elastic fracture mechanics models, continuum damage mechanics models and energy-based damage models (Kachanov, 1958, 1986; Rabotnov, 1969; Valanis, 1971, 1977; Chaboche, 1988; Murakami, 1988; Murakami and Kamiya, 1997; Onat and Leckie, 1988; Ju, 1989, 1990; Krajcinovic, 1989; Bazant, 1991; Chow and Chen, 1992; Lemaitre, 1996; Voyiadjis and Thiagarajan, 1996; Shi and Voyiadjis, 1997; Bonora and Newaz, 1998). Damage evolution function based on thermodynamics and statistical physics was first introduced by Basaran and Yan (1998) who established a relationship between entropy and damage for solids undergoing plastic deformations. Yet their model is not general enough to account for elastic deformations and to relate entropy production with material stiffness degradation.

There are many metrics to measure degradation in materials, such as direct measurements of the total crack areas lying on a surface, degradation of the elastic modulus, degradation of ultrasonic waves propagation speed, degradation of the microhardness, change in density, increase in electrical resistance, variation in the cyclic plastic response, change in creep properties, change in acoustic emission properties, remaining life and cumulative hysteresis energy. Damage process corresponding to the degradation of microstructure is, in general, irreversible. During the cumulative damage process, the internal entropy production, which is a measure of disorder in the system, must increase according to the second law of thermodynamics. So, internal entropy production can be used as a criterion for qualification of damage. Entropy in statistical physics and in the thermodynamic sense is really the same thing (Malvern, 1969). The statistical physics interpretation in terms of probability and tendency toward disordered microstates furnishes a physical significance for the otherwise rather abstract thermodynamic concept of entropy. Boltzmann (1898) first used statistical mechanics to give a precise meaning to the disorder and established a connection between the disorder and entropy for the whole system.

$$S = k_0 \ln W \tag{27}$$

where k_0 is Boltzmann constant and W is the disorder parameter which is the probability that the system will exist in the state relative to all the possible states it could be in. Statistical mechanics assigns an exact meaning to the probability of a state and supplies a general expression for W that employs the idea of the distribution function of a system. The relation between the entropy per unit mass and the disorder parameter is given by Basaran and Yan (1998):

$$s = \frac{R}{m_s} \ln W \tag{28}$$

where s is the entropy per unit mass, m_s is the specific mass, R is the gas constant. According to (28) we have the disorder function as follows:

$$W = e^{(m_s/R)s} \tag{29}$$

According to the second law of thermodynamics, all systems must fail when entropy is at maximum level and entropy production rate is zero. Hence the value of entropy at any time for all solid continuums, where the processes are always irreversible due to internal friction, identifies the level of degradation with respect to an initial point.

Let us define an isotropic damage variable D as the ratio of the change in disorder parameter to the current state disorder parameter with a proportional critical disorder coefficient D_{cr}:

$$D = D_{\mathrm{cr}} \frac{W - W_0}{W} = D_{\mathrm{cr}}\left[1 - e^{-(m_s/R)(s-s_0)}\right] \tag{30}$$

where W_0 is the disorder corresponding to the initial state of the continuous medium with entropy s_0. D_{cr} allows us to correlate the value of entropy production based damage D with other material coordinates, such as degradation of material stiffness. D_{cr} is easy to be determined from experimental data, but it can be different for different loading profiles such as monotonic and cyclic loading.

The fundamental equations governing the temperature, stresses, deformations and entropy production rate in a continuum medium have been derived in the previous section. From a strict viewpoint these quantities were all interrelated and had to be determined simultaneously. However, for most practical problems the effect of the stresses and deformations upon the temperature distribution is quite small and can be neglected. This procedure allows the determination of the temperature distribution in the solid resulting from prescribed thermal conditions to become the first and independent step of a thermal-stress analysis; the second step of such an analysis is then the determination of the stresses, deformations and damage in the body due to this temperature distribution (Boley and Weiner, 1988). Because the entropy change caused by the heat transfer between systems and surroundings has no influence on the degradation of the materials, only the entropy source strength, namely the entropy created in the system, should be used as a basis for the systematic description of the irreversible processes. So the damage evolution Equation (30) can be implemented in a numerical analysis procedure with the help of Equation (22) as follows:

$$s - s_0 = \int_{t_0}^{t} \frac{\boldsymbol{\sigma} : \underline{\varepsilon}^p}{T\rho} dt + \int_{t}^{t_0} \left(\frac{k}{T^2 \rho} \left|\mathrm{grad}\ T\right|^2 \right) dt + \int_{t_0}^{t} \frac{r}{T} dt \tag{31}$$

where the identity $\boldsymbol{\sigma} : \underline{\varepsilon} - \rho \dot{w}_{ava} = \boldsymbol{\sigma} : \underline{\varepsilon}^p$ is used, which represents the total mechanical dissipation rate. It should be pointed out that Equation (31) in conjunction with Equation (26) allows us to calculate the change in entropy (hence disorder) due to elastic deformations in the absence of plastic strains.

According to Equation (31), it is obvious that $D \geq 0$ is always satisfied because of the nonnegative entropy source strength. $D = 0$ when $\Delta s = 0$ and

$D = D_{\mathrm{cr}}$ when $\Delta s \to \infty$. Equation (31) shows that the damage is not only a function of the loading or straining process, but also of the temperature. However, a uniform increase in temperature in a stress free field does not cause any damage.

In order to simulate damage behavior of solid materials, there is a need for a progressive constitutive degradation model. Damage mechanics provides us a basic framework to develop damage evolution models at small strains. In accordance with the strain equivalence principle and Hook's law, the elasticity constitutive relationship may be written as (Lemaitre, 1996):

$$d\boldsymbol{\sigma} = (1 - D)\mathbf{C}_0\left(d\boldsymbol{\varepsilon} - d\boldsymbol{\varepsilon}^p - d\boldsymbol{\varepsilon}^T\right) \tag{32}$$

where $\mathbf{C}_0$ is the original stiffness matrix, $d\boldsymbol{\sigma}$ is the total stress increment vector, D is the isotropic damage parameter, $d\boldsymbol{\varepsilon}^T$ the incremental thermal strain, $d\boldsymbol{\varepsilon}^p$ is inelastic strain increment. If Von Mises type yield surface with isotropic and kinematic hardening is used in the constitutive model, the yield surface can be written according to the strain equivalence principle:

$$F = q^d - \bar{\sigma}^d \tag{33}$$

with the damage coupled back stress, equivalent Von Mises stress and yield stress defined as:

$$\alpha^d = (1 - D)\alpha \tag{34}$$

$$\bar{\sigma}^d = (1 - D)\bar{\sigma} \tag{35}$$

$$q^d = \sqrt{\frac{3}{2}(\mathbf{S} - \alpha^d) : (\mathbf{S} - \alpha^d)} \tag{36}$$

where $\mathbf{S}$ is the deviatoric stress tensor, α is the back stress tensor corresponding to kinematic hardening, $\bar{\sigma}$ is the tensile yield stress. The damage linearly decreases the yield stress, the isotropic strain hardening stress and the back stress.

It is emphasized that the following four equations, namely the fully coupled elastoplastic thermo-mechanical equation (26), the damage evolution function (30), the entropy production equation (31) and the constitutive relationship function (32) completely characterize the progressive damage behavior of any solid materials.

NUMERICAL SIMULATIONS AND EXPERIMENTAL COMPARISON

The model proposed in the previous sections is verified by implementing user subroutine into ABAQUS. The simulation results are compared with the corresponding strain-controlled monotonic tensile tests and fatigue tests on particulate composite prepared using lightly cross-linked poly-methyl methacrylate filled with alumina trihydrate, where the particle volume fraction is 48%.

It is well recognized that there is a very good correlation between the increase in crack density and the decrease in stiffness of the particulate composites. Thus, crack evolution under loads can be monitored by in situ stiffness measurements. This was framed in the theory of continuum damage mechanics with the scalar damage parameter D defined as (Kachanov, 1986):

$$D = 1 - \frac{E}{E_0} \tag{37}$$

where E is the instantaneous elastic module and E_0 is the initial value. This damage parameter was determined experimentally and compared with the proposed damage evolution function (30). The value of E is taken as that of the average unloading modulus in tension.

The geometry of the specimen used in the uniaxial tests is shown in Figure 1. Owing to the symmetry, only one half of the gauge length was used for simulation. To simulate the strain controlled uniaxial tests, the uniform displacement was applied to the end of the bar. For monotonic tensile tests, the maximum displacement is 0.9 mm. For the fatigue test the ramp displacement profile is shown in Figure 2. The material parameters needed for the proposed damage law are presented in Table 1.

Monotonic Tensile Tests

The Ramberg–Osgood plastic model was used to model the monotonic tensile plastic response, which is reasonably accurate for tensile behavior.

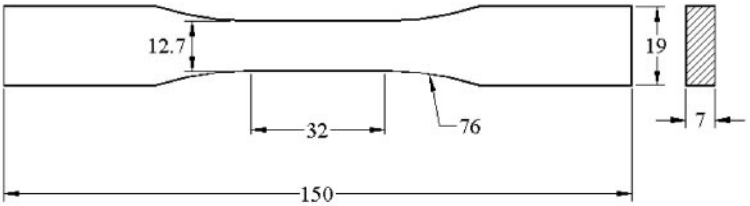

Figure 1. Uniaxial tensile test specimen geometry (mm).

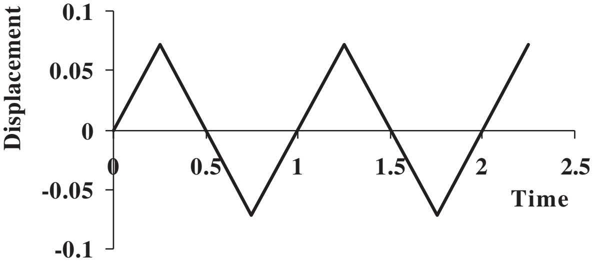

Figure 2. *Displacement profile for strain-controlled fatigue tests.*

Table 1. Material parameters.

Parameters	Values
Young's modulus (E)	10,000 MPa
Poisson's ratio (v)	0.35
Specific mass (m_s)	85 g/mole
Density (ρ)	1750 kg/m^3
Gas constant (R)	8.31451 J/mole/K
Temperature (T)	300 K

The constants $K = 295$ MPa and $n = 0.267$ for the Ramberg–Osgood model are easy to determine from experimental data near the yield point, where the damage is believed to be negligible. The constant $D_{\rm cr} = 130$ is used for monotonic loading. The stress–strain relationship obtained from the damage coupled plastic model is compared with the Ramberg–Osgood model and experimental data. The uniaxial tensile simulation versus Ramberg–Osgood plastic model and test data is shown in Figure 3. It is seen that the damage effects must be accounted for at relatively large strains and the proposed damage evolution function performs very well. The comparison of the damage parameter obtained from the damage coupled plastic model and that measured in experiments in terms of elastic modulus degradation is given in Figure 4. The simulation is in qualitative agreement with the experimental data.

Fatigue Tests

For simplicity, the linear kinematic hardening plastic model was used to model the fatigue response, which gives only a first approximation of the material behavior subjected to cyclic loading. Young's modulus $E = 8860$ MPa and hardening modulus $H = 31{,}147$ MPa for the linear kinematic

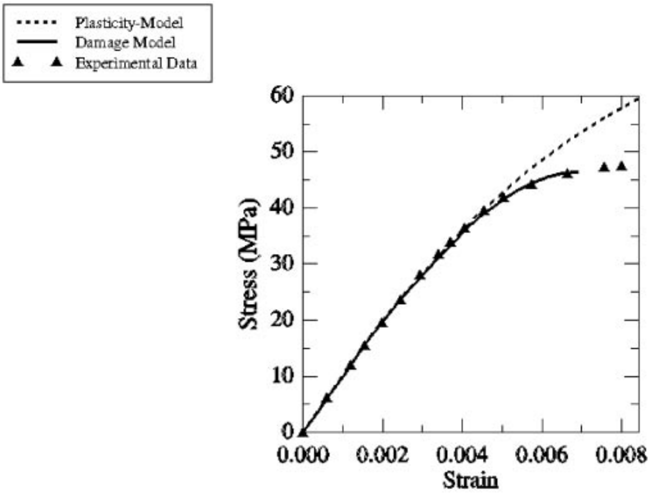

Figure 3. *Comparison of stress–strain relationship obtained from damage coupled plastic model with Ramberg–Osgood plasticity model and experiment data.*

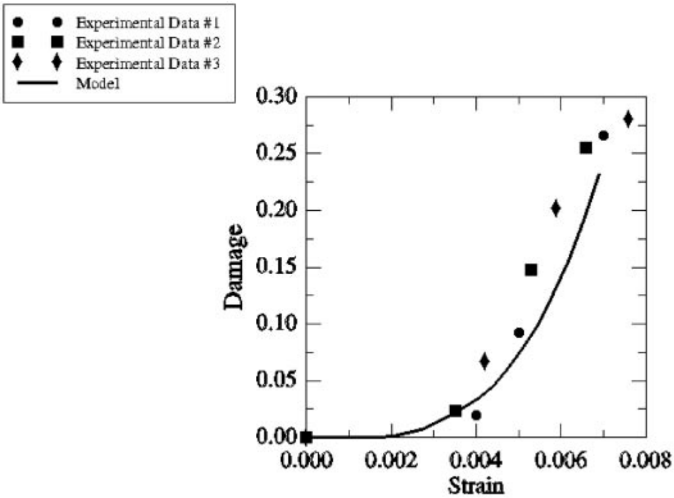

Figure 4. *Comparison of damage parameter obtained from damage coupled plastic model with that measured in experiments in terms of elastic modulus degradation.*

model are determined from experimental data in tension at the beginning of the 5th cycle, which is the stabilized cycle. The constant $D_{\mathrm{cr}} = 0.67$ is used for cyclic loading.

Comparisons of the uniaxial stress–strain hysteresis loop simulation with experimental data at cycle 5, 50 and 104 are shown in Figures 5, 6 and 7,

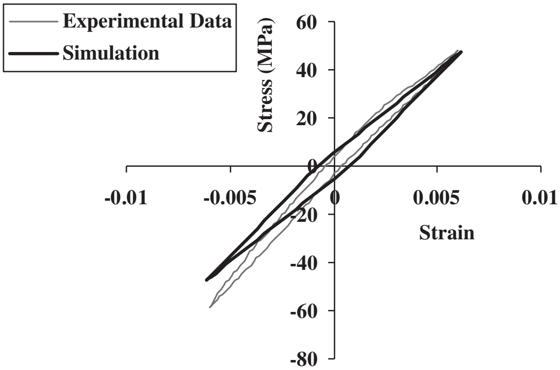

Figure 5. *Uniaxial stress–strain hysteresis loop simulation vs. experimental data at cycle 5.*

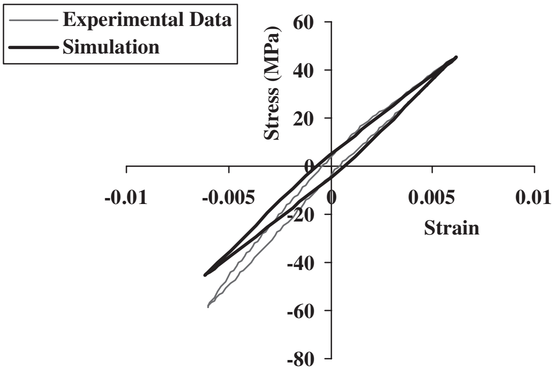

Figure 6. *Uniaxial stress–strain hysteresis loop simulation vs. experimental data at cycle 50.*

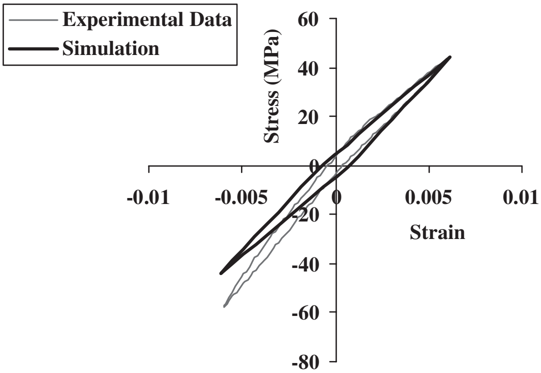

Figure 7. *Uniaxial stress–strain hysteresis loop simulation vs. experimental data at cycle 104.*

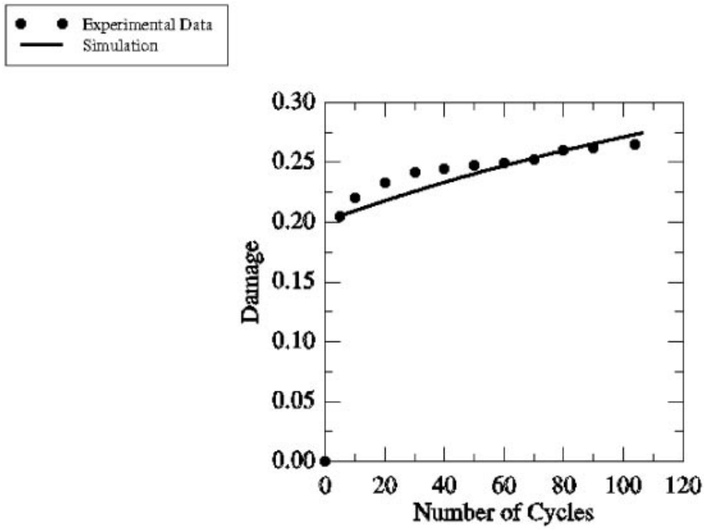

Figure 8. *Comparison of damage parameter obtained from damage coupled plastic model with that measured in experiments in terms of elastic modulus degradation.*

respectively. The proposed model performs very well except in compression. This is due to the values of parameters used in the model are measured in tension, but this kind of particulate composite exhibits markedly different inelastic behavior in tension and compression. The microstructure of particulate composite consists of a distribution of ATH flakes in a PMMA matrix. In tension, the ATH flakes act as stress concentrators, while in compression the flake serves to transmit stresses. The resulting material is brittle in tension, but in compression it is similar in behavior to PMMA.

The comparison of the damage parameter obtained from the damage coupled plastic model with that measured in experiments in terms of elastic modulus degradation is given in Figure 8. The simulation results are in good agreement with the experimental data. It is seen that most damage happens in the first few cycles, which is usually the reorganization of the initial manufacturing defects that can be introduced as initial damage in our model. Initial damage is probably due to the fact that particulate composites have many weak sites such as initial partial debonding between PMMA and ATH, agglomerates of ATH that dominate the damage experienced in the first few cycles.

The damage evolution law presented in this paper considers the damage as an isotropic internal state variable. This isotropic damage assumption is realistic in many cases especially under conditions of proportional loading when the principal stress directions remain unchanged (Lemaitre, 1996).

The comparison between the damage parameter measured in terms of elastic modulus degradation and simulation results from the damage evolution function validates that entropy can be used as a criterion for damage. The improvement of the proposed model over the Basaran and Yan (1998) model is that a critical damage coefficient D_{cr} is introduced to correlate disorder evolution with the material properties degradation. The proposed model also incorporates the fully coupled thermo-mechanical field equations, which allows the model to predict damage evolution from only elastic deformation loading cases.

CONCLUSIONS

An irreversible thermodynamic theory has been proposed for damage mechanics of solid materials. The proposed damage mechanics theory does not require any damage potential surface or an empirical Weibull function to trace the damage evolution in the material. Entropy production alone is used as a damage evolution metric for elastic and inelastic deformations. The proposed damage evolution equation can be used in conjunction with any material constitutive model and any vacancy (or void) generation model, including crystal plasticity and dislocation mechanics to initiate the microcracks at the smallest possible level. According to the theory proposed in this paper the influence of the microcracks initiating at multiple sites at dislocations level, can be bridged to macro level response by computing the entropy change of the macro system. Hence entropy production allows us to connect the atomic level behavior with macro-level response of the structure.

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