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**AN OVERVIEW OF A CONTINUUM  
MECHANIC APPROACH TO A  
THERMODYNAMIC MODEL OF FAILURE**

**Technical Report**

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The views expressed in this report are those of the authors and do not reflect the official policy or position of the Department of Defense or the U.S. Government

## ABSTRACT

This report provides a prelude to the work developed by Smirnov et al [1-4] considering the damage model of laminated composite materials. An overview of the thermodynamic definitions, concepts, and principles will be presented. This overview of the thermodynamics is necessary to provide the background needed to understand the damage model, which is based on thermodynamic principles. The essentials will be presented as follows: concepts and definitions, balancing laws, thermodynamic equilibrium or thermostatic, and the thermodynamic process. Furthermore, the essentials of the thermodynamics will be used to illustrate the development of the model of failure given by Kiselev and Yumashev [5]. The Kiselev and Yumashev model will be discussed prior to Smirnov's damage model since both are similar in their postulation of damage for structures undergoing impacts, and are based on thermodynamic principles. However, they are different in that the former is developed for elastoplastic isotropic homogenous material, and the latter is developed for laminated composite materials based on viscoelastic constitutive laws. That is, the constitutive equations for an elastoplastic material will be discussed to illustrate the use of a thermodynamic model of failure first, then the constitutive relations that incorporate a time dependent viscoelastic laminated composite materials will eventually be added in a subsequent report.

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# 1 INTRODUCTION

The writers are using this report as a overview to prepare the reader for the full work development of Smirnov et al [1-4] damage model for laminated composite materials. These references attempt to postulate a consistent damage model for laminated composite materials relating the deformation and failure under impact loading. In order to accomplish this, it becomes necessary to first consider a similar environment for isotropic materials [5]. In addition the failure, specifically the failure of a continuum under impact loading considered in references [1-5], is postulated as an energy dissipation criteria of a thermodynamic system in a time domain. Thus, the presentation of thermodynamic principles and related expressions used to postulate the thermodynamic model of failure become necessary to convey a clear picture of the model's development. In this way it is possible to appreciate all of the ramifications of various conditions which become relevant to an associated environment that actually present themselves in a thermodynamic model of failure, i.e. the flow of heat (heat flux), the continuum deformation, and finally the damage accumulation. Certain fundamental terms and relationships that will be encountered in the thermodynamic field must be examined thoroughly, e.g. specific free energy, internal energy, entropy, thermal flow, damage function, and stress-strain relationships. The writers, therefore, attempt to present a review of each of the fundamental topics required to understand the damage expressions published by Smirnov et al [1-4] for an impact type of problem. This overview, as an initial effort, will emphasize the expressions published by Kiselev and Yumashev [5] dealing with the deformation and failure of isotropic materials under impact. Note that in Kiselev and Yumashev [5], the constitutive equation models elastoplastic material under impact loading, however, in Smirnov et al [1-4] the constitutive equations model viscoelastic material under impact loading. As a first step, the Kiselev and Yumashev [5] constitutive equations for an

elastoplastic material will be discussed to illustrate the use of a thermodynamic model of failure. Further constitutive relations that incorporate a time dependent viscoelastic material will eventually be added.

The flow of ideas will be presented in the following form since the writers feel that an overall understanding of the failure model is only achieved by appreciating how the basic laws enter the global picture. A great deal of the actual mathematics for the relations can be found in Malvern [6], Maugin [7], and Mase and Mase [8], and relationships in these references will be used freely. The reader should consult these references for more details. It is our objective to show how the laws fit together, and how they are in general applied to a failure model. Thus, the following outline will be pursued:

1. The essentials of thermodynamics; a review of definitions, concepts, and principles of thermodynamics are presented. For clarity, this part is presented in four subsections as follows;
  - I. concepts and definitions; the writers will first review the essential concepts and definition of a thermodynamic system. These are important, since they establish the foundation used to formulate the principles of thermodynamics.
  - II. Balancing laws; they are the relationships that characterize the fundamental laws of a continuum. These laws are applicable to all material of a continuum and result in the governing equations that must be satisfied. They are presented in three parts, but they are intricately tied together:
    - A. the conservation laws dealing with mass, linear momentum, and angular momentum

for a purely mechanical system.

B. the heat conduction-convection for a system purely under heat transfer.

C. the first law and second laws of thermodynamics which are an energy balance of a system exchanging heat and work with its surroundings.

III. Thermodynamic equilibrium or thermostatic; a system under thermodynamic equilibrium or thermostatic state is defined, the governing laws are established, and the appropriate concepts for a thermostatic system are presented.

IV. Thermodynamic process; the concepts of a thermodynamic process is presented with two main presentations of the process; the axiomatic representation and the thermodynamics with internal variables representation.

2. The Thermodynamic model of failure; the thermodynamic model of failure presented by Kiselev and Yumashev [5] will be discussed in detail. This model uses thermodynamic concepts and principles, discussed in the section entitled "The Essential of Thermodynamics" to characterize failure of a continuum under impact loading.

## 2 THEORY

This theory section will be presented in two parts. The first part will review the essential elements of thermodynamics of a continuous homogenous media. The *definition* of the main concepts in thermodynamics and the principles governing a thermodynamic system will be presented. In this part, for example, thermodynamics quantities such as entropy, free energy, and enthalpy are defined, the first and second law that govern a thermodynamics system are presented, and the physical meaning of a thermodynamic process is interpreted. Once the concepts and principles of thermodynamics

are established, they will be used to characterize a thermodynamic model of failure since it is based on a thermodynamic approach that postulates failure as an energy dissipation mechanism in a time domain. The second part will establish the governing equations of a thermodynamic model of failure for a thermoelastoplastic medium. The model will be based on the thermodynamic principles that will be presented in the first section. The development of this model and the assumptions associated with it will be shown in detail using those established in the first section. The reader should consult Malvern [6], Maugin [7], and Mase and Mase [8], for more in-depth discussions of the postulations of thermodynamics.

Furthermore, it should be noted that continuum mechanic principles assume a continuous media which disregards gaps and empty spaces that might exist in the molecular structure of a matter. That is, it assumes that functions are well defined (i.e. continuously smooth and differentiable as many times as needed), and transformations are one-to-one (i.e. mappings are invertible and the Jacobian exist). In other words, the continuum mechanic principles are postulated under certain conditions or assumptions on the operators, functionals, and smoothness of domain and its boundary (i.e. nonsingular). This continuum mechanic theory does not consider special cases, such as sharp discontinuity of flow field variables, pressure, displacement, density, temperature due to shock wave and singularity of stress at the crack tip and discontinuity of displacement at the crack lips in fracture mechanics. In such special cases a theory is developed especially to model the physics of the problem, and the governing equations are derived specifically to incorporate the physics of that phenomena. For example, one way to model shock waves is the Rankine-Hugoniot relations for

changes across a shock. It is used to relate the flow immediately ahead of and behind the shock ( i.e. shock boundary condition), and the governing flow equations are used to calculate the remainder of the flow field between the shock and some other boundary condition, such as the surface of a body [9, 10]. Another way is to introduce artificial viscosity as a dissipating mechanism that would result in the shock wave being spread smoothly over a finite distance (i.e. several mesh grids in a computational discretization) [10]. Also, for a crack problem, i.e. macroscopic crack, the equilibrium equations, where the displacement at the crack is written in an asymptotic expansion form and the crack's boundary conditions are imposed, can be formulated leading to a stress' solution as a function of the distance ( $r$ ) from the crack tip [7]. This stress solution is proportional to the inverse of the square root of the distance from the crack tip (i.e. stress singularity at the crack tip is proportional to  $r^{-\frac{1}{2}}$ ).

This crack problem examines the damage mechanics of the continuum based on a macroscopic level where the crack more or less grows violently due to fatigue. Also, the damage mechanics in a continuum occurs on a microscopic level where a microcracks and microcavities caused by a damage process lead to a decrease in the material stiffness and strength (i.e. its ability to carry load is reduced). This microscopic damage process is of interest in this report since the thermodynamic model of failure discussed by Kiselev and Yumashev [5] is postulated based on the microscopic damage of the continuum. That is the microscopic damage process, which is initiated by impact loading, will cause an elastoplastic response in the material. This elastoplastic material response in a thermodynamic system is characterized as an irreversible thermodynamic process which is computed

qualitatively as an energy dissipation mechanism function of time (i.e. cumulative damage) that resulted from a high strain load.

## **2.1 Essential Elements of Thermodynamics**

In this section, the essential elements of thermodynamics are reviewed. To better present this section, it is divided into four subsection. The first will discuss *concepts* and *definitions* of terms that are used in the thermodynamic field. The second will show the *principles of thermodynamic* for both reversible and irreversible processes. The third, will discuss the laws of *thermodynamic equilibrium or thermostatics* associated with reversible thermodynamic processes. These laws are well established in the literature, and they will be used to represent the state of a thermodynamic system at a moment in time. Fourth, the *concept* of a thermodynamic process evolving from one state of thermodynamic equilibrium or thermostatic to another will be discussed.

### **I. Concepts and Definitions**

What is thermodynamics ? Thermodynamics is the science of studying energy and its relation to matter in a natural phenomena that is surrounding us, such as the motion of a pendulum, heating water, paddling a bicycle, and riding a roller coaster (these are simple examples). In other words, thermodynamics is the study of energy exchange of a well-defined geometrical volume as it evolves in time, i.e. change from one state to another. For example, and in simple terms, heating is adding energy to the water and paddling a bicycle is converting body energy into mechanical work. Note that, energy is a conceptual property, that is, a defined quantity used in postulating the laws of physics which exist in nature, and it is censored through its effects, i.e. to move an object from a point to another takes energy. A thermodynamic system is a system whose energy exchange with

the exterior is nothing but an exchange of heat and of work done. Such energy exchange could be recoverable or irrecoverable depending on the nature of the system being examined. For example, the amount of energy manifested in a bar that is loaded uniaxially could be recovered upon unloading for linear elastic material, that is the energy is conservative for a cyclic loading. However, if the load is increased such that the material reaches a nonlinear material response, then not all the energy is recoverable upon unloading or cyclic loading, and part of the energy is dissipated due to plasticity, viscoplasticity,...etc. Hence, to model these phenomena that exist in nature, there are two types of thermodynamics processes; reversible thermodynamics processes and irreversible thermodynamics processes.

A reversible thermodynamics process, such as a pendulum under gravitational force and friction free, the oscillation of mass connected to an elastic spring, (i.e. undamped vibration), compression of an ideal gas, and an elastic collisions of two balls, are processes where the kinetic and potential energy may be fully transformed from one state to the other in the absence of a dissipation mechanism (i.e. energy proceed from kinetic to potential energy and visa versa in a cycle). The state of a reversible thermodynamics process is referred to as a state of equilibrium, thermostatic or thermodynamic equilibrium interchangeably, and its governing principles are well established in the literature and will be summarized later.

An irreversible process is a nonconservative process due to some sort of energy dissipation, which is not recoverable, such as viscous force, friction, and nonlinear response of material. An irreversible

phenomena often occurs in conditions removed far from equilibrium (i.e. a process does not exhibit equilibrium in a thermostatic sense as in a reversible process) where linear constitutive equations are no longer applicable for thermodynamic inputs. Even though an irreversible thermodynamic process, in its main sense, is the study of a phenomena outside a state of equilibrium, an irreversible thermodynamic process is conceived as a transition from one state of equilibrium to another. Thus, it is the study of phenomena outside a state of equilibrium, but in the vicinity of an equilibrium state, so that some of the concepts and principles developed for a state of equilibrium of a reversible process can be assumed to be applicable during the evolving of an irreversible thermodynamic process in time. Numerically, this concept allows for an incremental approach. This concept will be revisited later.

Before proceeding with the discussion of the principle that govern the physics of a thermodynamic process, first some important concepts which will allow us to better understand the physical meaning of these principles are presented, such as energy, heat, and work. What is energy ? Energy is a conceptual property defined to explain interactions between systems. For example, a molecule possess energy by virtue of their translation through space, which is called microscopic kinetic energy. This kinetic energy, which molecules possess, could be due to translational, rotational, vibrational, or spinning motion of the molecules. Also, molecules are held together by molecular binding forces, and the concept of potential energy is associated with these intermolecular forces. The macroscopic internal energy is the total energy possessed by the molecules. For example, applying an external uniaxial load to a bar of a linear elastic material causes intermolecular forces inside the bar which

are proportional to the potential energy per unit mass  $\hat{u}$  (i.e. the so-called specific strain energy) defined as

$$\hat{u} = \int_0^{\epsilon_{ij}} \sigma_{ij} d\epsilon_{ij} \quad (1)$$

where  $\sigma_{ij}$  is a stress tensor and  $\epsilon_{ij}$  is a strain tensor. For a continuum in motion, the macroscopic kinetic energy  $\mathbf{K}$  of a system is the energy associated with the macroscopically observable velocity  $\mathbf{v}$  of the continuum, and it is defined as

$$\mathbf{K} = \int_V \frac{1}{2} \rho \mathbf{v} \cdot \mathbf{v} dV, \quad (2)$$

where  $\rho$  is density (i.e. mass per unit volume),  $\mathbf{v}$  is a velocity vector. In this report, the convention adopted is that a bold symbols indicate tensors of first order and higher (i.e. vectors and tensors). Note that an isolated system is one where the energy for the system is constant and no change of energy occurs.

It was mentioned earlier that a thermodynamic system is a system whose energy exchange with the exterior is nothing but an exchange of heat and work. What is heat and work ? Heat is the amount of energy being transferred between two systems having two different temperatures. That is, considering two adjacent systems  $A$  and  $B$  at two different temperatures that are capable of exchanging energy, the heat will flow between the two systems carrying energy from the hotter to the colder systems until their temperature are balanced. The time rate of the heat flow is called flux or heat flux. Note that an isothermal system is one where its temperature is constant and does not change, and a system that is under going an adiabatic deformation is one where no heat transfer is

allowed. Note that heat flux can not be measured directly, but its effects can be indirectly observed, such as melting of ice, and the warming and vaporization of water. The concept of work which could be mechanically moving an object a distance  $\delta$  by applying a force  $F$ , compressing gas's volume  $dV$  by applying a pressure  $p$ , or changing the state of an electrical charge  $dQ$  by applying a voltage  $\hat{V}$ , ...etc., can be expressed in a general equation as

$$\hat{W} = \int_0^{\hat{\alpha}_i} \hat{\tau}_i d\hat{\alpha}_i, \quad \text{where } i = 1 \dots n, \quad (3)$$

where  $\hat{W}$  is the work,  $\hat{\alpha}_i$  represents the quantitative change of an  $i$ th degree of freedom, and  $\hat{\tau}_i$  is the conjugate of the  $i$ th quantitative change  $\hat{\alpha}_i$ . The word conjugate means a pair, and it is used in general to relate quantities that act in pairs to produce some sort of energy, such as force and displacement, volume and pressure in gases, voltage and electrical charge,...etc. Power is defined as the time rate of work. Note that work and heat are unlike energies, which are stored within matter. Heat and work are not stored within matter, but they are two ways to transfer energy across the boundary. That is, doing work (supplying power) and transferring heat (supplying heat flux) to a system increases the amount of energy stored within matter for that system.

Furthermore, how is the state of a system characterized ? In general, a state of a system is characterized by a real finite set of quantities that are determined by the physics of the system (i.e. experimentally proper to that system), whether of geometric, mechanical, thermal, electrical, physicochemical,...etc. in nature. Note that one draws from experiment that only a limited number of these quantities, which are properties of the physical state of the continuum, are mutually independent. Also, mutually independent quantities are sufficient to characterize the physical state of

the system. Mutually independent quantities are also required to impose a well-defined mathematical system where the physical state of the system is invariant, i.e. the physical state is independent of the choice of these mutually independent quantities. For example, in solid mechanics to describes the deformation of a body under mechanical loading, either loads or displacements are chosen to characterize the physical state of the system since they are related by the constitutive equations. In either case, the solution is independent of the quantities chosen to characterize the system, and the choice is influenced by the approach being used to model and solve the problem. Also, to describe the physical state of a given quantity of an ideal gas, its pressure, specific volume, and temperature could be used to characterize the physical state of the system, however, only two are mutually independent (i.e. independent variables) since there exist gas law equations that relate pressure, specific volume, and temperature.

In a thermodynamic system, the continuum is characterized by macroscopic quantities, which are mutually independent, and they are called state variables. These state variables can be scalar, vectorial, or tensorial such as temperature, an anisotropic damage parameter, strain tensor,...etc., and in a general formulation, they are left arbitrary, i.e.  $\alpha$  for a scalar quantity,  $\alpha_i$  for a vector quantity, and  $\alpha_{ij}$  for a tensor quantity. Within a homogenous system (a homogenous system is one that has properties at all points that are the same), the state variables are said to be *extensive* if they are proportional to the mass of the system; in general the total amount of an extensive variable in the system is proportional to the total mass. Otherwise, they are an *intensive* state variable which means they do not depend on the mass of the system in equilibrium; in general the point

value of an intensive variable does not depend on the size of the system. For example, entropy is an extensive variable conjugate to the intensive variable temperature. However, a *specific intensive* state variable is an extensive state variable per unit mass. For example, the specific internal energy is an intensive quantity equal to the internal energy per unit mass. A subset of the state variables is called substate variables. The choice of the state variables is determined by the physical nature of the system, its transformation, and the scheme adopted to characterize the material response, so that the state variables may change from one system and theory to another.

The next question is how is the material modeling of the thermodynamic continuum established? The material modeling for a thermodynamic continuum can be divided into three areas; constitutive model, state equation, and failure model. First, the constitutive model characterizes the material and its reaction to load, such as elastic, elastic-plastic, and viscoplastic for stress-strain response in solid mechanics and Newtonian and Non-Newtonian for stress versus rate of deformation response in fluid mechanics. Second, the equation of state is an experimental or derived relationship which express a macroscopic quantity that is characteristic of the a thermodynamic system in terms of the state variables. For example, the internal energy for a thermodynamic solid continuum can be expressed in term of the state variables; entropy and strain tensor. Also, for Newtonian fluid, internal energy can be expressed in term of the state variables, which are temperature and density. Third, a failure model provides a criterion predicting its initiation and describing its growth in a continuum. For example, the microscopic damage that occurs in a continuum due to high strain load reduces the ability of the material to carry load, and could be characterized parametrically in terms of the

dissipating energy as being postulated by Kiselev and Yumashev [5]. Their failure model will be presented later in detail with the type of material modeling being used in their model.

Finally, the different representations used to describe the evolution process of a system (i.e. the process through time) is presented. There are two possible types of descriptions for the governing equations independent of the coordinate system; **Lagrangian** and **Eulerian** descriptions. That is the independent variables, which describe a state equation of a particle, are either with respect to a fixed coordinate system, i.e. **Lagrangian**, or a moving coordinate system with the particle, i.e. **Eulerian** (see Figure 1). In a Cartesian coordinate system for example, the change in a particle's Cartesian position vector in a Lagrangian formulation  $d\mathbf{X}$  is described with respect to the original configuration which is fixed in time (i.e. the Cartesian coordinate system at time  $t = 0$ ), and the change in a particle's Cartesian position vector in an Eulerian formulation  $d\mathbf{x}$  is described with respect to the present configuration which is moving with the particle (i.e. the Cartesian coordinate system at time  $t$ ) (see Figure 1). Note that, the position vector  $\mathbf{x}$  is used with Eulerian description and the position vector  $\mathbf{X}$  is used with Lagrangian description. Also, note that the coordinate system that will be used in the formulation is the Cartesian coordinate system in this report.

The **Lagrangian** and **Eulerian** representations have the following differences in the equation formulation. First, Lagrangian and Eulerian representations lead to a different time derivative that will depend on whether a Lagrangian description or an Eulerian description is used (see Malvern [6],

chapter 4). That is the time derivative of a function  $f$  in a Lagrangian description is

$$\dot{f}(\mathbf{X}, t) = \frac{\partial f}{\partial t}, \quad \text{or} \quad \frac{D}{Dt} = \frac{\partial}{\partial t}, \quad (4)$$

and the time derivative of a function  $f$  in an Eulerian description is

$$\dot{f}(\mathbf{x}, t) = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial \mathbf{x}} \cdot \mathbf{v}, \quad \text{or} \quad \frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{x}}, \quad (5)$$

where  $\mathbf{v}$  is the velocity vector of the particle at time  $t$ , and  $\frac{D}{Dt}$  is another conventional form that is used in the literature. That is the time derivative  $\frac{D}{Dt}$  defined in Equation (4) for a Lagrangian formulation is equal to the time derivative  $\frac{\partial}{\partial t}$ , and the time derivative for an Eulerian formulation defined in Equation (5) consist of two derivatives, the time derivative of a fixed point  $\frac{\partial}{\partial t}$  and the rate of change due to the movements of coordinate system (i.e. attached with the moving particle)  $\mathbf{v} \cdot \frac{\partial}{\partial \mathbf{x}}$ . Note that, a time derivative  $\frac{D}{Dt}$  for an Eulerian description reduces to

$$\frac{D}{Dt} = \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{x}}, \quad (6)$$

for steady state, and reduces to

$$\frac{D}{Dt} = \frac{\partial}{\partial t}, \quad (7)$$

for a uniform state, (i.e. no change or variation). In the remainder of this report, the time derivative  $\frac{D}{Dt}$  of a variable ( $a$ ), for example, will be replaced by  $\dot{a} = \frac{Da}{Dt}$ , that is

$$\dot{a} = \frac{Da}{Dt} = \frac{\partial a}{\partial t} + \mathbf{v} \cdot \frac{\partial a}{\partial \mathbf{x}}, \quad (\text{ for Eulerian formulation } ), \quad (8)$$

$$\dot{a} = \frac{Da}{Dt} = \frac{\partial a}{\partial t}, \quad (\text{ for Lagrangian formulation } ), \quad (9)$$

Second, the type of stress and strain tensors used in each formulation are different. For a Lagrangian formulation, the stress tensor is the second Piola-Kirchhoff stress tensor  $P_{IJ}$  and Green strain tensor  $L_{IJ}$  (see Figure 2). The Green strain tensor  $L_{IJ}$  is applicable for problems with large displacements and rotations. But, in an Eulerian formulation, the stress tensor is the Eulerian stress tensor  $T_{ij}$  and Almansi's strain tensor  $E_{ij}$  (see Figure 2). The Almansi's strain tensor  $E_{ij}$  is also applicable for problems with large displacements and rotations. Note that the indices  $I$  and  $J$  are used to indicate Lagrangian description and the indices  $i$  and  $j$  are used to indicate Eulerian description. Furthermore, if an incremental approach is used where large displacement might exist, an infinitesimal response for the stress-strain due to infinitesimal strain-displacement relations can be used. Thus, the stress and strain tensors, for both the Eulerian and Lagrangian formulation, reduce to the Cauchy stress tensor  $\sigma_{ij}$  and the Cauchy strain tensor  $\epsilon_{ij}$ , respectively. These are referred to as the incremental Cauchy stress tensor  $d\sigma_{ij}$  and Cauchy strain tensor  $d\epsilon_{ij}$  (i.e. an up-dated Lagrangian approach is incorporated numerically). In addition, in a rate dependent problem such as the elastic-plastic problem, where the rigid body rotations of a material point undergoing deformation is assumed that it does not affect deformations, an incremental approach must be used, and infinitesimal stress-strain response also can be used (i.e. the incremental Cauchy stress and strain tensors). However, to eliminate the rigid body rotations from the material point deformation, the Jaumann stress rate is used. The details of the Jaumann stress rate will be discussed later in the thermodynamic model of failure section.

Finally, note that, the use of **Lagrangian** description or **Eulerian** description is dominated by

the physics of the problem. For example, the former is widely used in solid mechanics since the history of a material under going deformations is important, and it is measured with respect to the original configuration. While the latter is widely used in fluid mechanics since the flow of the material at an instant is important. Hence, it is measured with respect to a coordinate system moving with the flow. A detail comparison between the Eulerian and Lagrangian formulation can be found in Anderson [10] which outline the difference between the two mathematical descriptions (e.g. the mass, momentum, and energy flow into and out of the cell where the volume is invariant in the Eulerian formulation compared to the fixed mass of a grid moving relative to a fixed coordinate system in the Lagrangian formulation) and their numerical solution (e.g. for Lagrangian mesh boundary conditions, free surfaces and contact surfaces are straightforward compared with the Eulerian approximate material interfaces and exterior boundaries, however the distortion of the Lagrangian mesh as the grid moves is no longer an issue in the fixed Eulerian grid).

## II. Balancing Laws

A continuum, which is undergoing mechanical, thermal, or thermomechanical process is governed by balancing equations. For, example, considering an elastic structure which is statically loaded, the forces for any segment of the structure or the entire structure are balanced by the equilibrium equation. In the case of dynamic loading, the balancing laws for the structure are the equations of motion. The general forms of the balancing laws for a mechanical process are the conservation laws, which are the conservation of mass, conservation of linear momentum and conservation of angular momentum. For a thermal process, they are the heat conduction-convection equations. For a thermodynamic system where mechanical energies are being exchanged within the system, the balancing

equations are the energy balance equations or the so-called two principles of thermodynamics; the first law and second law of thermodynamics. These laws postulate the energy balance for a system which are the energies carried in or out of the system by means of work and heat, or the energy generated by the system as it evolves from one state to another. Since, mechanical work and heat transfer relationships are the bases of thermodynamic system, and they are commonly used in many practical applications in the field of engineering, these relationships will be summarized first leading to the thermodynamic principles. Hence, the three systems are presented in the following order: a purely mechanical system followed by a purely thermal system and finally a thermodynamic system. Also, both Eulerian and Lagrangian representations will be shown in the formulations of the balancing laws for the sake of completeness.

First, for a purely mechanical system (i.e. adiabatic and isothermal system) the governing equations are the conservation laws of a continuum of a volume  $V$  bounded by a surface  $S$ . These conservation laws are the governing equations of a mechanical system that insure mechanical balance for the continuum (i.e. equivalent to equilibrium equations for a continuum under static state and equations of motion for a continuum under dynamic state, respectively). These governing equations, combined with other equations such as constitutive equations and boundary conditions, are used to compute quantities related to the deformation of a continuum under mechanical load, such as a displacement field, stress field, strain field,.....etc. in a continuum. The Eulerian formulation will be presented first then the Lagrangian formulation, and these conservation laws can be summarized as:

- The conservation of mass, also called the **Continuity equation**, states that no mass is created

or destroyed inside a volume  $V$ . That is, the inflow of mass through element  $dS$  is equal to the rate of increase of the total mass. This can be expressed in an integral form (see Figure 3) as

$$-\int_S \rho v_n dS = \int_V \rho_{,t} dV , \quad (10)$$

where  $\rho(\mathbf{x}, t)$  is the density as function of position (space) and time  $t$ ,  $(\ )_{,t} = \frac{\partial(\ )}{\partial t}$  is the partial derivative with respect to time,  $v_n$  is the outward normal component of the velocity vector  $\mathbf{v}(\mathbf{x}, t)$  ( i.e.  $v_n = \mathbf{v} \cdot \mathbf{n}$ ),  $\mathbf{n}$  is the outward normal, and the negative sign is present since the inflow of mass is used (i.e. the normal component of the velocity vector is negative in the inflow case,  $\mathbf{v} \cdot \mathbf{n} = -v_n$ ). Using the **Divergence theorem**, (**Gauss's theorem**), which states that the integral of the outer normal component of a vector ( $a$ ) over a closed surface is equal to the integral of the divergence of the vector over the volume bounded by the closed surface, i.e. in vector notation,

$$\int_S \mathbf{a} \cdot \mathbf{n} dS = \int_V \nabla \cdot \mathbf{a} dV , \quad (11)$$

where the gradient  $\nabla$  of a scalar function at a point is defined as the normal vector to the function at that point, and its expression is given as

$$\nabla = \frac{\partial}{\partial x} \hat{\mathbf{i}} + \frac{\partial}{\partial y} \hat{\mathbf{j}} + \frac{\partial}{\partial z} \hat{\mathbf{k}} , \quad (12)$$

and  $\hat{\mathbf{i}}, \hat{\mathbf{j}}$ , and  $\hat{\mathbf{k}}$  are the Cartesian's basis vectors. Or in indicial notation, the divergence theorem is

$$\int_S a_i n_i dS = \int_V a_{i,i} dV , \quad (13)$$

where  $a_{,i} = \frac{\partial a}{\partial x_i}$  is the partial derivative of the vector  $\mathbf{a}$  with respect to  $i$ th component of

Cartesian position vector  $\mathbf{x}$ . Then the continuity equation, Equation (10), reduces to

$$-\int_V \nabla \cdot (\rho \mathbf{v}) dV = \int_V \rho_{,t} dV , \quad (14)$$

$$-\int_V (\rho_{,i} v_i + \rho v_{i,i}) dV = \int_V \rho_{,t} dV , \quad (15)$$

$$\int_V (\rho_{,t} + \rho_{,i} v_i + \rho v_{i,i}) dV = 0 . \quad (16)$$

Hence, the conservation of mass equation per unit volume is equal to

$$\rho_{,t} + \rho_{,i} v_i + \rho v_{i,i} = 0 , \quad ( \text{Eulerian} ) , \quad (17)$$

or presented differently,

$$\dot{\rho} + \rho v_{i,i} = 0 , \quad ( \text{Eulerian} ) , \quad (18)$$

where  $\dot{\rho}$  is the time derivative of the density  $\frac{D\rho}{Dt}$  defined in Equation (8) and it is

$$\dot{\rho} = \frac{D\rho}{Dt} = \rho_{,t} + \rho_{,i} v_i , \quad (19)$$

Note that, for an incompressible material, the density of the material remain constant, and Equation(18) becomes

$$v_{i,i} = 0 . \quad (20)$$

Equation (20) is the compressibility conditions where the divergence of the velocity is zero and it is representative of fluid particle with a velocity  $\mathbf{v}$ . For a solid representation, Equation (20) can be written (see Malvern [6], chapter 4) as

$$v_{i,i} = \dot{\epsilon}_{ii} = \frac{\dot{V}}{V} = 0 . \quad (21)$$

In some materials the elastic response is essentially incompressible (e.g. rubber), but this is not usually the case. However, for inelastic material, it is often assumed to be approximately

incompressible, such as metals undergoing plastic flow. The plasticity theory assumes plastic incompressibility which indicates that plasticity does not cause volume change (i.e. no dilatational change since deviatoric stresses, which are the stress tensor minus the hydrostatic pressure, are used in the plasticity theory), but it causes plastic deformation due to a dislocation of the crystallographic planes in metals. Thus, plastic incompressibility is assumed in this report and for the thermodynamic model of failure where a plastic constitutive model for metals is used.

Similarly, the Lagrangian formulation for the conservation of mass is

$$\dot{\rho} = 0 , \quad ( \text{Lagrangian} ) , \quad (22)$$

This Lagrangian formulation of the conservation of mass state that the density of an original volume (i.e. at time  $t = 0$ ) remain constant as the system evolves in time.

Note that the continuity equation is a valid assumption for continuous and discontinuous media (e.g. shock waves and fracture mechanics) which assumes mass is neither created nor destroyed in the system. However for the latter, i.e. discontinuous media, a state equation or failure model describing the discontinuity in the continuum is necessary. For example, considering the spalling phenomena which occurs in high velocity impact, a failure criteria modeling spalling is necessary where the debris and the laws governing its behavior are accounted for in the

modeling and the conservation of total mass of the total system (i.e. the remains of the continuum and the debris) is satisfied.

- The conservation of linear momentum states that the time rate of the change of the total linear momentum of a given system is equal to the vector sum of all the external forces acting on the system provided that Newton's third law of action and reaction governs the internal forces. For an incompressible material, the conservation of linear momentum expressed in an integral form (see Figure 4) is

$$\int_S \mathbf{t} dS + \int_V \rho \mathbf{b} dV = \int_V \rho \dot{\mathbf{v}}_i dV , \quad (23)$$

where  $\mathbf{t}(\mathbf{x}, t)$  is the traction vector, and  $\mathbf{b}(\mathbf{x}, t)$  is the body force per unit mass. Also, the traction vector can be written in terms of the stress tensor  $T_{ij}$  and normal vector  $\mathbf{n}$  (Cauchy's law) as

$$\mathbf{t} = \mathbf{T} \cdot \mathbf{n} , \quad (24)$$

or in indicial notation,

$$t_i = T_{ij} n_j , \quad (25)$$

and using the divergence theorem, the conservation of linear momentum reduces to

$$\int_V (T_{ij,j} + \rho b_i) dV = \int_V \rho \dot{v}_i dV , \quad (26)$$

that is

$$T_{ij,j} + \rho b_i = \rho \dot{v}_i , \quad (\text{Eulerian}) . \quad (27)$$

This is also called Cauchy's equations of motion and they are the governing equations of a mechanical system (i.e. the system is mechanically balanced). In Equation (27), the equilibrium is for a displaced point where stresses are acting on the undeformed area along the orthogonal coordinate axis that translate with the material point, i.e. the Eulerian stress tensor  $T_{ij}$ .

Similarly, the Lagrangian formulation for the conservation of linear momentum can be written as

$$P_{I,J} + \rho b_I = \rho \dot{v}_I , \quad ( \text{Lagrangian} ) , \quad (28)$$

where  $( )_{,I} = \frac{\partial}{\partial X_I}$ , i.e. the partial derivative with respect to the position in the Lagrangian description and the  $dV$  and  $dS$  are in the original coordinate system. In Equation (28), the equilibrium is for a displaced point where stresses are acting on the deformed area, i.e. second Piola-Kirchhoff stress tensor  $P_{IJ}$ .

- The conservation of angular momentum states that time rate of the change of the total angular momentum of a given system is equal to the vector sum of the moments of all the external forces acting on the system. Expressed in an integral form (see Figure 5), the conservation of angular momentum equation is

$$\int_S \mathbf{r} \times \mathbf{t} dS + \int_V \rho \mathbf{r} \times \mathbf{b} dV = \int_V \rho (\mathbf{r} \times \dot{\mathbf{v}}) dV , \quad (29)$$

where  $\mathbf{r}$  is the moment arm with respect to the center of coordinate system center (i.e. the position vector). Using indicial notation, the conservation of angular momentum equation

becomes

$$\int_S e_{kij} x_i t_j dS + \int_V e_{kij} x_i b_j dV = \int_V \rho e_{kij} (x_i \dot{v}_j) dV , \quad (30)$$

where  $e_{kij}$  is the permutation symbol. Expressing the traction in term of Eulerian's stress tensor  $T_{ij}$ , Equation (25), and the divergence theorem, the integral form of the conservation of angular momentum, Equation (29), becomes

$$\int_v e_{kij} (x_i T_{j1,l} + x_{i,l} T_{j1}) dV + \int_V e_{kij} x_i b_j dV = \int_V \rho e_{kij} (\dot{x}_i v_j + x_i \dot{v}_j) dV . \quad (31)$$

But,  $x_{i,l}$  is equal to the Kronecker delta  $\delta_{il}$  (i.e.  $x_{i,l} = \delta_{il}$ ),  $\dot{x}_i$  is equal to the velocity  $\dot{x}_i = v_i$ , and  $e_{kij} v_i v_j = 0$  by definition since it is symmetric in term of the indices  $i$  and  $j$ . Hence, the above equation reduces to

$$T_{ij} = T_{ji} . \quad (32)$$

That is the Eulerian's stress tensor is symmetric.

Similarly, the Lagrangian formulation for the conservation of angular momentum can be written as

$$P_{IJ} = P_{JI} , \quad ( \text{Lagrangian} ) , \quad (33)$$

which indicates that the second Piola-Kirchhoff stress tensor  $P_{IJ}$  is symmetric. Again note that the  $dV$  and  $dS$  shown in Figure 5 is in the original coordinate system even though the quantities of stress are on the deformed body.

The second set of balancing laws relates to heat transfer which is the theory that refers to heat flux and the temperature in continuum with respect to time and no mechanical deformation. The governing equations for a homogeneous isotropic body based on heat balance for a given differential volume is formulated as follows. For a given differential volume, the heat balance must be conservative such that the difference between the heat flow in minus the heat flow out through the surface of the differential volume is balanced by the heat within the differential volume (i.e. generated or lost) which is equal to the heat change of the differential volume ( $c\dot{\theta}$ ), where  $c$  is the specific heat defined as the quantity of heat required to raise the temperature of a unit mass one degree and  $\theta$  is the temperature (see Figure 6). That is

$$\begin{aligned} & (q_x - q_x - q_{x,x})dA_x + (q_y - q_y - q_{y,y})dA_y + \\ & (q_z - q_z - q_{z,z})dA_z + \rho r_h(x, y, z, t) = \rho c \dot{\theta} dV , \end{aligned} \quad (34)$$

where  $dA_x$ ,  $dA_y$ , and  $dA_z$  are the area of the  $x$ ,  $y$ , and  $z$  faces in the Eulerian formulation, respectively, of the differential volume,  $q_x$ ,  $q_y$ , and  $q_z$  are the heat flux vector through the  $x$ ,  $y$ , and  $z$  faces, respectively,  $r_h(\mathbf{x}, t)$  is the heat source or sink per unit mass function of position and time, and it is the heat generated inside the continuum, such as electrical resistance heating inside the body, chemical reaction (for example epoxy and concrete generate heat when curing), or radiation due to nuclear, microwave, electromagnetic, or others. Similarly, for a given differential volume in the Lagrangian formulation, the heat balance is

$$\begin{aligned} & (q_x - q_x - q_{x,x})dA_x + (q_y - q_y - q_{y,y})dA_y + \\ & (q_z - q_z - q_{z,z})dA_z + \rho r_h(X, Y, Z, t) = \rho c \dot{\theta} dV , \end{aligned} \quad (35)$$

where  $dA_x$ ,  $dA_y$ , and  $dA_z$  are the undeformed area of the  $X$ ,  $Y$ , and  $Z$  faces in the Lagrangian

formulation, respectively, of the differential volume,  $q_x$ ,  $q_y$ , and  $q_z$  are the heat flux vector through the  $X$ ,  $Y$ , and  $Z$  faces, respectively after deformation based on the undeformed area and volume,  $r_h(\mathbf{X}, t)$  is the heat source or sink per unit mass function of position and time. Dividing Equations (34) and (35) by the differential volume  $dV$  and taking the limit ( $dV \rightarrow 0$ ), the above conduction-convection equations can be written as

$$q_{i,i} + \rho r_h = \rho c \dot{\theta} , \quad (\text{Eulerian}) , \quad (36)$$

$$q_{I,I} + \rho r_h = \rho c \dot{\theta} , \quad (\text{Lagrangian}) . \quad (37)$$

Furthermore, assuming that the heat flux obeys Fourier's law of heat conduction for a homogeneous and isotropic material, which assumes that the heat flux is proportional linearly to the temperature gradient, that is

$$q_i = -k \theta_{,i} , \quad (\text{Eulerian}) , \quad (38)$$

$$q_I = -\bar{k} \theta_{,I} , \quad (\text{Lagrangian}) , \quad (39)$$

where  $k$  and  $\bar{k}$  are the thermal conductivity of the body. the heat flux in the Eulerian and Lagrangian representation are related through

$$q_I = J_a \mathbf{F} q_i , \quad (40)$$

$$\theta_x = J_a \frac{k}{\bar{k}} \mathbf{F} \theta_x , \quad (41)$$

where  $\mathbf{F}$  is the deformation gradient matrix,  $J_a$  is the determinant of the deformation gradient matrix or the so-called the Jacobian, and if the thermal conductivity is for isotropic material and assumes that it is independent of position and temperature, one can set ( $k = \bar{k}$ ) since the thermal conductivity of a body is scalar for isotropic material. For Eulerian or Lagrangian representation,

either the governing equations (36) or (37), respectively, combined with Fourier's law equation gives a partial differential equations for the temperate field. Imposing the boundary conditions of the system, the solution of the temperature field is obtained from these governing partial differential equations.

Third, now that the two cases where either work or heat are exchanged with a system (i.e. the analysis of mechanical work and heat transfer are decoupled) has been discussed, the thermodynamic case where the system's exchange of work and heat are coupled will be presented next. Thermodynamics analyzes a system where both work and heat are exchanged with a system. That is, thermodynamics analyzes a system where mechanical work and heat transfer are coupled. Thus, the thermodynamic principles that govern a system postulate the energy balance of a system undergoing both mechanical work and heat exchange with its surrounding as the system evolves in time from one state to another. These principles are the first law and second law of thermodynamics, and they will be presented as follows:

The first law of thermodynamics is an energy balance law between the stored energy in the continuum and the energies being exchanged with the system through its surrounding (i.e. the work done on the system and the heat transfer into the system). That is, the first law of thermodynamic is the relation in which the total time rate of change in energy (kinetic and internal is balanced by the total energy exchanged by work and heat through the surrounding. The energy balance of a

thermodynamic system expressed in mathematical form is

$$\dot{\mathbf{K}} + \dot{\mathbf{E}} = \dot{\mathbf{P}} + \dot{\mathbf{Q}} , \quad (42)$$

where  $\mathbf{E}$  is the internal energy and  $\dot{\mathbf{E}}$  is the time rate of change in the internal energy,  $\mathbf{K}$  is the kinetic energy and  $\dot{\mathbf{K}}$  is the time rate of change in the kinetic energy,  $\mathbf{P}$  is the mechanical work input generated by the traction  $\mathbf{t}$  acting on the surface of the continuum and the body forces  $\mathbf{b}$  acting on the continuum and  $\dot{\mathbf{P}}$  is the time rate of change in the work which is also called the power input, and  $\mathbf{Q}$  is the heat input and  $\dot{\mathbf{Q}}$  is time rate of change in the heat input which consists of the heat supplied to the continuum by the heat flux vector  $\mathbf{q}$  through the surface, and the internal heat source (or sink) distributed per unit mass  $r_h$  inside the continuum. These time rate quantities  $\dot{\mathbf{E}}$ ,  $\dot{\mathbf{K}}$ ,  $\dot{\mathbf{P}}$ , and  $\dot{\mathbf{Q}}$  are defined as

$$\begin{aligned} \dot{\mathbf{E}} &= \frac{D}{Dt} \int_V \rho u dV , & \dot{\mathbf{K}} &= \frac{D}{Dt} \int_V \frac{1}{2} \rho \mathbf{v} \cdot \mathbf{v} dV , \\ \dot{\mathbf{P}} &= \int_S \mathbf{t} \cdot \mathbf{v} dS + \int_V \rho \mathbf{b} \cdot \mathbf{v} dV , & \dot{\mathbf{Q}} &= \int_S \mathbf{q} \cdot \mathbf{n} dS + \int_V \rho r_h dV , \end{aligned} \quad (43)$$

respectively, where  $u$  is the internal energy per unit mass (i.e. specific internal energy), and  $\mathbf{n}$  is a normal unit vector which is positive in the outward direction. Substitute Equations (43) into equation (42) produces

$$\frac{D}{Dt} \int_V \frac{1}{2} \rho \mathbf{v} \cdot \mathbf{v} dV + \frac{D}{Dt} \int_V \rho u dV = \int_S \mathbf{t} \cdot \mathbf{v} dS + \int_V \rho \mathbf{b} \cdot \mathbf{v} dV + \int_S \mathbf{q} \cdot \mathbf{n} dS + \int_V \rho r_h dV . \quad (44)$$

Then, writing the traction in term of the Eulerian's stress tensor  $T_{ij}$ , i.e. Cauchy's law in Equation (25), and using divergence theorem, the above equation reduces to

$$\int_V \rho \dot{u} dV = \int_V \left[ \frac{1}{2} (v_{i,j} + v_{j,i}) T_{ij} + \rho r_h - q_{i,j} \right] dV , \quad (45)$$

or in a tensor field form (per unit volume),

$$\rho \dot{u} = T_{ij} D_{ij} + \rho r_h - q_{i,j} , \quad ( \text{ Eulerian } ) , \quad (46)$$

where the tensor  $\mathbf{D}$  is the so-called rate of deformation tensor or the stretching tensor, which is a symmetric tensor and defined as

$$D_{ij} = \frac{1}{2}(v_{i,j} + v_{j,i}) , \quad ( \text{ Eulerian } ) . \quad (47)$$

Note that, the stretching tensor in Equation (47) is used in fluid mechanics, but in solid mechanics the partial derivative of the velocity with respect to space coordinates, i.e.  $v_{i,j}$  is expressed as a strain rate (i.e.  $v_{i,j} = \dot{E}_{ij}$  for Eulerian representation), and the stretching tensor  $\mathbf{D}$  reduces to

$$D_{ij} = \dot{E}_{ij} , \quad ( \text{ Eulerian } ) . \quad (48)$$

The stretching tensor in Equation (48) will be used in the development of the thermodynamic model of failure which is applicable to homogenous isotropic metal. Also, the quantity  $(T_{ij} D_{ij})$  is a tensor product defined as

$$\mathbf{T} : \mathbf{D} = T_{ij} D_{ij} , \quad (49)$$

where the symbol  $:$  represent a tensor product and  $(\mathbf{T} : \mathbf{D})$  is the so-called stress power which is the rate of work generated by the traction. Equation (46) provides the sufficient relation to insure the energy balance required by the first law of thermodynamic (i.e. an energy balance between work, heat, kinetic energy, and internal energy) for the continuum at all times.

Similarly, the Lagrangian formulation for the first law of thermodynamic is

$$\rho \dot{u} = P_{IJ} D_{IJ} + \rho r_h - q_{I,J} , \quad ( \text{Lagrangian} ) , \quad (50)$$

where the tensor  $D_{IJ}$  is the Lagrangian formulation of the rate of deformation tensor or the stretching tensor, which is a symmetric tensor and defined as

$$D_{IJ} = \frac{1}{2}(v_{I,J} + v_{J,I}) , \quad ( \text{Lagrangian} ) , \quad (51)$$

and the tensor product  $(P_{IJ} D_{IJ})$  is the stress power,

$$\mathbf{P} : \mathbf{D} = P_{IJ} D_{IJ} , \quad ( \text{Lagrangian} ) , \quad (52)$$

Furthermore, in solid mechanics the partial derivative of the velocity with respect to the coordinates is expressed as a strain rate (e.g.  $v_{I,J} = \dot{L}_{IJ}$ ), and the stretching tensor  $\mathbf{D}$  reduces to

$$D_{IJ} = \dot{L}_{IJ} , \quad ( \text{Lagrangian} ) . \quad (53)$$

It was mentioned earlier that if an incremental approach is used to solve the problem, then infinitesimal strain-displacement assumption can be used even if large displacements exist in the problem. In this case, incremental Cauchy's stress and strain tensors ( $d\sigma_{ij}$  and  $d\epsilon_{ij}$ ) are used. That is, both the Green and Eulerian strain tensors reduce to the incremental Cauchy's strain tensor. Also, the second Piola-Kirchhoff stress tensor and the Eulerian stress tensors reduce to the incremental Cauchy's stress tensor. Furthermore, the Eulerian and Lagrangian form of the stretching tensors become equal ( $D_{ij} = D_{IJ}$ ) also the stress power in Eulerian and Lagrangian formulations become equal to  $(\sigma_{ij} \epsilon_{ij})$ .

The first law of thermodynamic can be regarded as an expression of the interconvertibility (i.e. the internal process that a continuum manifest as a reaction to the energy being exchanged through its surrounding in order to balance the system's total energy by converting different forms of energy that are exchanged and stored internally) of heat and work maintaining an energy balance, and it places no restriction on the thermodynamic process, i.e. reversible and irreversible. The second law of thermodynamics postulate the existence of entropy  $\eta$  per unit mass and further places restriction on an irreversible thermodynamic process. What is entropy ? Entropy, like internal energy, is a conceptual property, and it is extensive in the sense that the entropy of a system is the sum of all its parts. The entropy property is involved in the energy flow term unlike the internal energy which is involved in the energy storage term. That is entropy is the change of heat energy exchanged with the system and hypothetically, a system going for a full cycle, a reversible process does not generate entropy as it return to its initial state. However, for an irreversible process as the system is going through a full cycle, an internal entropy is created by the system which is always positive and can not be destroyed. That is, entropy is the heat energy added or subtracted to the continuum for a reversible processes, and it is the heat energy added, subtracted, and generated by the continuum for irreversible processes. Thus, for a system going for a full cycle, a reversible process does not generate entropy, but an irreversible process does, and this energy generated by irreversible process can not be destroyed. A significant increase in entropy is viewed as a reduction in the system's ability to do efficient work and a change of entropy becomes a parametric way to characterize the efficiency of a process. For a scientists and engineers, a reversible process is more efficient in doing work than irreversible one , however, in nature most thermodynamic processes are irreversible, and it is the engineers job to provide the most efficient process possible. For example, Carbon has lower entropy

in the form of a diamond, which is a hard crystal with atoms closely bound in a highly ordered form, than it has as graphite (see Kubaschewski and Evans [11]). In other words, entropy provides a means to characterize the efficiency of a thermodynamic system's interconvertibility of heat and work maintaining an energy balance. A system that is undergoing an isentropic deformation is a one where the change of entropy is zero, i.e. the entropy of the system is constant. The entropy for a reversible and irreversible thermodynamic process will be presented separately.

In a reversible process, entropy as a state variable is defined by the state function,

$$d\eta = \left( \frac{dQ_m}{\theta} \right)_{rev}, \quad (54)$$

where  $dQ_m$  is the change in heat input per unit mass, and  $\theta$  is the absolute temperature. Note that, absolute temperature is a temperature measured on an absolute scale, which is chosen in this case as Kelvin scale to avoid division by zero. In this case, entropy is a perfect differential ( $\oint d\eta = \oint \left( \frac{dQ_m}{\theta} \right)_{rev} = 0$ ). That is, the kinetic and potential energy may be fully transformed from one to the other in the absence of a dissipation mechanism (i.e. can equally proceed in either direction, that is potential energy to kinetic energy or kinetic energy to potential energy, such as the case of freely swinging pendulum in the absence of friction, where the energy proceeds from kinetic to potential energy as the pendulum swings upwards and from potential to kinetic energy as the pendulum swings downwards in a cycle).

For an irreversible process, entropy is not a perfect differential ( $\oint \left( \frac{dQ_m}{\theta} \right)_{rev} \neq 0$ ) and the **Clausius-**

**Duhem** inequality postulate these irreversible processes (see Malvern [6], chapter 5). Clausius-Duhem inequality states that for an irreversible process, changing from state 1 to state 2 due to heat transfer input  $dQ_m$ , the entropy increase is greater than the entropy input by heat transfer,

$$d\eta \geq \int_1^2 \left( \frac{dQ_m}{\theta} \right)_{irrev} . \quad (55)$$

That is, for an irreversible thermodynamic process, the system's entropy for a cycle due to heat input is ( $\oint d\eta = 0$ ), which mean that for a cycle the total entropy resulting from the heat transfer input  $dQ_m$  and the entropy produced by the continuum due to an irreversible process (e.g. plastic deformation) are characterized as conservative. However, the change in heat flow  $dQ_m$  for a continuum in a cycle is not ( $\oint \left( \frac{dQ_m}{\theta} \right)_{irrev} \neq 0$ ) since it does not account for the heat generated by the irreversible process, i.e. the heat dissipation mechanism of a system undergoing the irreversible process. For example, contact friction and plastic flow in solid mechanic dissipate heat in addition to the heat transfer being exchange through the system boundary. This is modeled by the Clausius-Duhem inequality which states that the total time rate of change in entropy per unit mass is never less than the supplied entropy through heat. In other words modeling the nonconservative process of heat transfer by imposing a restriction on the irreversible of a thermodynamic process). Thus, dividing Equation (55) by  $dt$ , mathematically reduces it to a rate form,

$$\dot{\eta} \geq \left( \frac{\dot{Q}_m}{\theta} \right)_{irrev} . \quad (56)$$

Multiply Equation (56) by the density and integrate over the volume, Equation (56) becomes

$$\int_V \rho \dot{\eta} dV \geq \int_V \rho \left( \frac{\dot{Q}_m}{\theta} \right)_{irrev} dV . \quad (57)$$

But, the inequality's right hand side integral is the rate of the heat input (i.e.  $\dot{Q} = \int_V \rho \left( \frac{\dot{Q}_m}{\theta} \right)_{irrev} dV$ ).

Substitute the values of the rate of the heat input given in Equation (43), and using the divergence

theorem, lead to the following

$$\int_V \rho \dot{\eta} dV \geq \int_S \frac{1}{\theta} \mathbf{q} \cdot \mathbf{n} dS + \int_V \frac{1}{\theta} \rho r_h dV , \quad (58)$$

$$\int_V \rho \dot{\eta} dV \geq \int_V \left[ \left( \frac{q_i}{\theta} \right)_{,i} + \frac{1}{\theta} \rho r_h \right] dV , \quad (59)$$

where

$$\left( \frac{q_i}{\theta} \right)_{,i} = \frac{1}{\rho \theta} q_{i,i} - \frac{1}{\rho \theta^2} \theta_{,i} q_i ,$$

and the state equation of the second law of thermodynamic (for a unit volume) reduces to

$$\dot{\eta} - \frac{r_h}{\theta} + \frac{1}{\rho \theta} q_{i,i} - \frac{1}{\rho \theta^2} \theta_{,i} q_i \geq 0 , \quad ( \text{ Eulerian } ) \quad (60)$$

The first term in Equation (60) is the rate of change of the total entropy, the second term is the rate of change of entropy due to heat source or sink, and the third and fourth terms are the rate of change of entropy due to heat flux. The left hand of the inequality is called the dissipation function  $d$  and it represents the energy dissipation of an irreversible process which is always positive (e.g. plasticity). Thus, Equation (60) can be expressed as

$$d = \dot{\eta} - \frac{r_h}{\theta} + \frac{1}{\rho \theta} q_{i,i} - \frac{1}{\rho \theta^2} \theta_{,i} q_i \geq 0 , \quad \text{or} \quad d \geq 0 \quad ( \text{ Eulerian } ) . \quad (61)$$

Similarly, the Lagrangian formulation for the second law of thermodynamic is

$$\dot{\eta} - \frac{r_h}{\theta} + \frac{1}{\rho \theta} q_{I,I} - \frac{1}{\rho \theta^2} \theta_{,I} q_I \geq 0 , \quad ( \text{ Lagrangian } ) , \quad (62)$$

$$d_I = \dot{\eta} - \frac{r_h}{\theta} + \frac{1}{\rho \theta} q_{I,I} - \frac{1}{\rho \theta^2} \theta_{,I} q_I \geq 0 , \quad \text{or} \quad d \geq 0 \quad ( \text{ Lagrangian } ) , \quad (63)$$

where  $d_l$  is the Lagrangian counterpart of the Eulerian's dissipation function  $d$ . The terms in Equation (62) are in the Lagrangian form where the first term is the rate of change of the total entropy, the second term is the rate of change of entropy due to heat source or sink, and the third and fourth terms are the rate of change of entropy due to heat flux.

### III. Thermodynamic Equilibrium or Thermostatic

The concepts and terminologies of a thermodynamic equilibrium or thermostatic state will be discussed in this section. The words thermodynamic equilibrium and thermostatic refer to a reversible thermodynamic process and they are used interchangeably. This is different from a non-equilibrium thermodynamic process, which is postulated as a process transiting from one state of thermodynamic equilibrium or thermostatic to another. Hence, it is necessary to present the thermodynamic equilibrium or thermostatic state first leading to a thermodynamic process, and thus the relation between the thermostatic and thermodynamic processes will be discussed in detail in the next section.

The thermodynamic equilibrium or thermostatic is associated with the principle that govern a reversible thermodynamic process. The reversible thermodynamic process occurs in conditions where linear constitutive equations are applicable and where equilibrium (i.e. the physical state of a system is balanced between the internal and external elements using an equality) is satisfied. For example, the entropy defined in equation (54) satisfy equilibrium where the change of entropy equals the change of heat input divided by the absolute temperature. Also, in this section, the concept of

thermodynamic potential which will be used in developing the thermodynamic model of failure later will be defined for a thermostatic system. These thermodynamic potentials are the internal energy, free energy and enthalpy of a thermostatic system, and they will be presented as follows:

First, the internal energy defined for a thermostatic state assumes that the thermodynamic equilibrium system is based on the **caloric** equation of state (see Malvern [6], chapter 5). The caloric equation of state assumes that the local internal energy  $u$  per unit mass is determined by the thermodynamic state specified by the entropy  $\eta$  and the  $n$ th substate variable ( $\alpha_i$ ,  $i = 1..n$ ), by definition. In the general formulation, these substate variables are arbitrary, and they have mechanical or electromagnetic dimensions. Their choice depend on the physical nature of the system and the scheme adopted to describe the system, and will be specified later. Thus, in mathematical form, the caloric equation of state is stated as

$$u = u(\eta, \alpha, \mathbf{x}) , \quad ( \text{ Eulerian } ) , \quad (64)$$

$$u = u(\eta, \alpha, \mathbf{X}) , \quad ( \text{ Lagrangian } ) , \quad (65)$$

where the internal energy is a state function, i.e. depending on position vector which is either  $\mathbf{x}$  in an Eulerian formulation or  $\mathbf{X}$  in a Lagrangian formulation, and it is characterized by the state variables  $\eta$  and  $\alpha$ . From the definition of the internal energy in the caloric equation of state for a thermostatic (see Malvern [6], chapter 5), the thermodynamics absolute temperature  $\theta$  and the thermodynamic tensions  $\tau_i$  which are the conjugate of the substate variables  $\alpha_i$ , are given as

$$\theta \equiv \left( \frac{\partial u}{\partial \eta} \right)_{\alpha} , \quad \tau_i \equiv \left( \frac{\partial u}{\partial \alpha_i} \right)_{\eta} , \quad i = 1, 2, \dots, n \quad (66)$$

where the subscripts outside the parentheses indicate variable held constant. In other words, Equation (66) gives a mathematical definition for thermodynamics absolute temperature  $\theta$  and the thermodynamic tensions  $\tau_i$  in term of the internal energy that is defined based on the caloric equation of state. Note that, the thermodynamic tensions  $\tau_i$  is the conjugate of the substate variables  $\alpha_i$ , and they will be used in the definitions of thermodynamic potential. For example, considering an ideal gas, a substate variable is the volume and its conjugate is the pressure where a change in volume causes pressure change and visa versa a change in pressure causes change in volume.

Further, for a reversible thermodynamic process, combining the first law and second law of thermodynamic leads to the so-called **Gibbs** relation (see Malvern [6], chapter 5),

$$du = \theta d\eta + \tau_i d\alpha_i . \quad (67)$$

Using the corollary of **Carnot's** theorem (see Maugin [7], appendix 1) which state that a thermodynamic system can always be described by the state variables  $(\{\eta, \alpha_1, \dots, \alpha_i, \dots, \alpha_n\}; i = 1, \dots, n)$ , in such a way that

$$\kappa = \theta d\eta, \quad \omega = \tau_i d\alpha_i , \quad (68)$$

where  $\kappa$  is the so-called elementary heat received by the continuum for a reversible process, and it is the heat energy exchanged by the system, and  $\omega$  is the so-called elementary work in a reversible process and, it is the energy transferred through the work performed by the thermodynamic tensions  $\tau_i$  due to substate variables' change  $d\alpha_i$ , one can rewrite the Gibbs relation Equation (67) as

$$du = \kappa + \omega , \quad (69)$$

which shows the Gibbs relation as an energy balance equation of heat and work that govern a thermostatic state.

The thermodynamic tension could be related to the stress tension as follow. Considering a special case of a recoverable adiabatic and isentropic deformation, the **Gibbs** relation, Equation (67), reduces to

$$du = \tau_i d\alpha_i , \quad (70)$$

and divide both sides by  $(dt)$ , the rate form equation is obtained as

$$\dot{u} = \tau_i d\dot{\alpha}_i . \quad (71)$$

Also, the Eulerian and Lagrangian representations of the first law of thermodynamic, Equations (46) and (50), respectively, reduce to

$$\dot{u} = \frac{1}{\rho} T_{ij} D_{ij} , \quad ( \text{ Eulerian } ) , \quad (72)$$

$$\dot{u} = \frac{1}{\rho} P_{IJ} D_{IJ} , \quad ( \text{ Lagrangian } ) . \quad (73)$$

Also, the rate of deformation can be expressed in term of the rate of strain, which is compatible to the solid mechanics representation. That is, in the case where the substate variables (i.e. the tensor form of the state variables  $\alpha_{ij}$ ) are equal to Eulerian's strain tensor  $E_{ij}$  for an Eulerian representation and Green's strain tensor  $L_{ij}$  for a Lagrangian representation, and their conjugates (i.e. the tensor form of the thermodynamic tension  $\tau_{ij}$ ), the Eulerian's stress tensor  $T_{ij}$  and the second Piola-Kirchhoff stress tensor  $P_{IJ}$ , respectively, the rate of deformation tensor is equal to the

rate of the strain tensor as,

$$D_{ij} = \dot{E}_{ij} , \quad ( \text{ Eulerian } ) , \quad (74)$$

$$D_{IJ} = \dot{L}_{IJ} , \quad ( \text{ Lagrangian } ) , \quad (75)$$

respectively. Equating Equations (71) and Equation (72) for Eulerian formulation and equating Equations (71) and Equation (73) for Lagrangian formulation show that the work of the thermodynamic tensions is recoverable and equal to the external stress power defined in Equations (49) and (52),

$$T_{ij} D_{ij} = \rho \tau_{ij} \dot{\alpha}_{ij} , \quad ( \text{ Eulerian } ) , \quad (76)$$

$$P_{IJ} D_{IJ} = \rho \tau_{IJ} \dot{\alpha}_{IJ} , \quad ( \text{ Lagrangian } ) , \quad (77)$$

Replacing the state variables  $\alpha_{ij}$  by the proper strain tensor (i.e. Eulerian or Green strain) and using the rate of deformation given in Equations (74) and (75), the thermodynamic tensions  $\tau_{ij}$  reduce to

$$\tau_{ij} = \frac{T_{ij}}{\rho} , \quad \text{where } \alpha_{ij} = E_{ij} , \quad ( \text{ Eulerian } ) . \quad (78)$$

$$\tau_{ij} = \frac{P_{ij}}{\rho} , \quad \text{where } \alpha_{ij} = L_{ij} , \quad ( \text{ Lagrangian } ) . \quad (79)$$

Note that there is a difference between the two stresses in Equations (78) and (79), where in the former the stress is acting on an undeformed area at the present displaced points while the latter stress is acting on a deformed area with respect to the original coordinates.

Furthermore, for isotropic and homogenous thermoelasticity continuum the stress and strain tensors are linear elastic stress (i.e. the thermoelasticity is consistent with the infinitesimal assumption), and they are equal to the incremental Cauchy's stress tensor  $d\sigma_{ij}$  and incremental Cauchy's

strain  $d\epsilon_{ij}^e$  (i.e. consistent with up-dated Lagrangian assumption). Setting the substate variables equal to Cauchy's strain tensor ( $\alpha_{ij} = \epsilon_{ij}^e$ ) and replacing the second Piola-Kirchhoff stress tensor  $P_{IJ}$  and the Eulerian stress tensor  $T_{ij}$  by Cauchy's stress tensor  $\frac{\sigma_{ij}}{\rho}$  in Equations (78) and (79)), the substate conjugate  $\tau_{ij}$  reduces to ( $\tau_{ij} = \frac{\sigma_{ij}}{\rho}$ ). Choosing entropy and Cauchy's strain tensor as state variables, the internal energy  $u(\eta, \epsilon_{ij}^e)$  can be expressed as,

$$u(\eta, \epsilon_{ij}^e) = \frac{\lambda}{2} \epsilon_{kk}^e{}^2 + \mu \epsilon_{ij}^e \epsilon_{ij}^e - \frac{K \alpha_v \theta_0}{c_\epsilon} \epsilon_{kk}^e \eta + \theta_0 \eta + \frac{\theta_0}{2c_\epsilon} \eta^2, \quad (\text{Thermoelasticity}) \quad (80)$$

and its incremental form is

$$du = \lambda \epsilon_{kk}^e d\epsilon_{kk}^e + 2\mu \epsilon_{ij}^e d\epsilon_{ij}^e - \frac{K \alpha_v \theta_0}{c_\epsilon} (\epsilon_{kk}^e d\eta + \eta d\epsilon_{kk}^e) + \theta_0 d\eta + \frac{\theta_0}{c_\epsilon} \eta d\eta, \quad (\text{Incremental}) \quad (81)$$

where  $\lambda$  and  $\mu$  are the Lamé's constant,  $K$  the bulk modulus or volumetric modulus,  $\alpha_v$  the coefficient of linear volume expansion,  $c_\epsilon$  the specific heat at a constant strain, and  $\theta_0$  is the temperature at the natural state or the initial absolute temperature. Note that, Equation (80) is obtained by expanding the internal energy into the Taylor series in the vicinity of the natural state of strain and entropy retaining only up to second order terms (see Nowacki [12] for full details). Substituting the internal energy for a thermoelastic medium (Equation (80)) into Equation (66), the temperature and Cauchy's stress can be expressed as

$$\theta \equiv \left( \frac{\partial u}{\partial \eta} \right)_\alpha = -\frac{K \alpha_v \theta_0}{c_\epsilon} \epsilon_{kk}^e + \theta_0 + \frac{\theta_0}{c_\epsilon} \eta, \quad (\text{Thermoelasticity}) \quad (82)$$

$$\frac{\sigma_{ij}}{\rho} \equiv \left( \frac{\partial u}{\partial \epsilon_{ij}^e} \right)_\eta = \lambda \delta_{ij} \epsilon_{kk}^e + 2\mu \epsilon_{ij}^e - \frac{K \alpha_v \theta_0}{c_\epsilon} \delta_{ij} \eta, \quad (\text{Thermoelasticity}). \quad (83)$$

and their incremental forms are

$$d\theta = -\frac{K \alpha_v \theta_0}{c_\epsilon} d\epsilon_{kk}^e + \theta_0 + \frac{\theta_0}{c_\epsilon} d\eta, \quad (\text{Incremental}) \quad (84)$$

$$\frac{1}{\rho} d\sigma_{ij} = \lambda \delta_{ij} d\epsilon_{kk}^e + 2\mu d\epsilon_{ij}^e - \frac{K \alpha_v \theta_0}{c_\epsilon} \delta_{ij} d\eta, \quad (\text{Incremental}). \quad (85)$$

Note that, the internal energy and the relations that follow from it for a thermoelastic system characterize the thermostatic state, and they will be used as a part of the development of the thermodynamic model of failure which assumes that an irreversible thermodynamic process is a transition from one thermostatic state to the other (i.e. one can view a non-equilibrium thermodynamic processes as one that consist of a thermostatic state as it evolves in time). This will become evident as the thermodynamic model of failure is discussed in detail later.

Second, based on the assumed caloric equation of state being used, the internal energy  $u$  per unit mass is a thermodynamic potential. Another form of thermodynamic potential is the **free energy** or the so-called Helmholtz free energy  $\psi$  (see Malvern [6], chapter 5). It is defined as the portion of the internal energy available for doing work at a constant temperature, that is

$$\psi(\theta, \alpha) = u - \eta\theta . \quad (86)$$

Note that the first term in Equation (86) is the total internal energy, and the second term is an energy term representing the internal energy due to heat exchange. For example, consider isentropic deformation (i.e.  $\eta = 0$ ), then the free energy is equal to the internal energy and for an elastic continuum the free energy is equal to the potential energy which is given in Equation (1). Based on the free energy as a thermodynamic potential, the entropy and the thermodynamic tension, that is similar to Equation (66), can be written as

$$\eta \equiv -\left(\frac{\partial\psi}{\partial\theta}\right)_{\alpha} , \quad \tau_i \equiv \left(\frac{\partial\psi}{\partial\alpha_i}\right)_{\theta} , \quad i = 1, 2, \dots, n . \quad (87)$$

In other words, Equation (87) gives a mathematical definition for entropy  $\eta$  and the thermodynamic

tensions  $\tau_i$  in terms of the free energy (see Malvern [6], chapter 5).

Using the free energy definition in Equation (86), the Gibbs relation (Equation (67)) becomes

$$d\psi = -\eta d\theta + \tau_i d\alpha_i . \quad (88)$$

Note that the independent variables used in the internal energy  $u(\eta, \alpha)$  are the entropy  $\eta$  and the substate variables  $\alpha_i$ , but in the free energy  $\psi(\theta, \alpha)$  the independent variables used are the absolute temperature  $\theta$  and the substate  $\alpha_i$ . Hence, the choice of using the thermodynamic potentials depends on which state variable are chosen to characterize a thermodynamic system.

Considering a special case of an isothermal deformation with reversible heat transfer, that is

$$\begin{aligned} d\theta &= 0 , \\ \dot{\eta} &= \frac{1}{\theta} \left( r_h - \frac{1}{\rho} q_{i,i} \right) , & \text{( Eulerian ) ,} \\ \dot{\eta} &= \frac{1}{\theta} \left( r_h - \frac{1}{\rho} q_{I,I} \right) , & \text{( Lagrangian ) ,} \end{aligned} \quad (89)$$

where  $r_h$  is the internal heat source (or sink) distributed per unit mass inside the continuum, then the **Gibbs** relation (Equation (88)) reduces to

$$d\psi = \tau_i d\alpha_i , \quad (90)$$

and divide both sides by  $dt$ , the rate form of the equation is

$$\dot{\psi} = \tau_i d\dot{\alpha}_i . \quad (91)$$

Also, eliminating the internal energy in the first law of thermodynamic Equations (46) and (50), i.e. the Eulerian and Lagrangian representations, respectively, in term of the free energy defined in Equation (86), and substituting the value of  $\dot{\eta}$  defined in Equation (89) for a reversible heat transfer, the following relation are deduced

$$\dot{\psi} = \frac{1}{\rho} T_{ij} D_{ij} , \quad (\text{ Eulerian } ) , \quad (92)$$

$$\dot{\psi} = \frac{1}{\rho} P_{IJ} D_{IJ} , \quad (\text{ Lagrangian } ) . \quad (93)$$

Expressing the rate of deformation in terms of the strain rate tensor where the choice of a substate variables (i.e. the tensor form of the state variables  $\alpha_{ij}$ ) are equal to Eulerian's strain tensor  $E_{ij}$  for an Eulerian representation and Green's strain tensor  $L_{ij}$  for a Lagrangian representation, it become equal to

$$D_{ij} = \dot{E}_{ij} , \quad (\text{ Eulerian } ) , \quad (94)$$

$$D_{IJ} = \dot{L}_{IJ} , \quad (\text{ Lagrangian } ) , \quad (95)$$

respectively. Equating Equations (91) and Equation (92) for Eulerian representation and (93) for Lagrangian representation shows that the work of the thermodynamic tensions is recoverable and equal to the external stress power defined in Equations (49) and (52), respectively,

$$T_{ij} D_{ij} = \rho \tau_{ij} \dot{\alpha}_{ij} , \quad (\text{ Eulerian } ) , \quad (96)$$

$$P_{IJ} D_{IJ} = \rho \tau_{IJ} \dot{\alpha}_{IJ} , \quad (\text{ Lagrangian } ) , \quad (97)$$

Replacing the substate variables  $\alpha_{ij}$  by the strain tensor and use the rate of deformation tensor given in Equations (94) and (95), the thermodynamic tensions  $\tau_{ij}$  reduce to the stress tensors as,

$$\tau_{ij} = \frac{T_{ij}}{\rho} , \quad \text{where} \quad \alpha_{ij} = E_{ij} , \quad (\text{ Eulerian } ) . \quad (98)$$

$$\tau_{IJ} = \frac{P_{IJ}}{\rho}, \quad \text{where } \alpha_{IJ} = L_{IJ}, \quad (\text{Lagrangian}). \quad (99)$$

Note that there is a difference between the two stresses in Equations (98) and (99), where in the former the stress is acting on an undeformed area at the present displaced points while the latter, the stress is acting on a deformed area with respect to the original coordinates.

It was mentioned earlier that the stress and strain tensors for an isotropic and homogenous thermoelasticity continuum are linear elastic stress and strain tensors. If an incremental approach is used to solve the problem, then infinitesimal strain-displacement assumption can be used even if large displacements exist in the problem. That is, both the Green and Eulerian strain tensors reduce into Cauchy's strain tensor. Also, the second Piola-Kirchhoff stress tensor and the Eulerian stress tensors reduce to Cauchy's stress tensor. Thus, in the up-dated Lagrangian approach the stress and strain tensors are the incremental Cauchy's stress tensor  $d\sigma_{ij}$  and the incremental Cauchy's strain tensor  $d\epsilon_{ij}^e$ . Setting the substate variables equal to Cauchy's strain tensor ( $\alpha_{ij} = \epsilon_{ij}^e$ ) and replacing the second Piola-Kirchhoff stress tensor  $P_{IJ}$  and the Eulerian stress tensor  $T_{ij}$  by Cauchy's stress tensor  $\frac{\sigma_{ij}}{\rho}$  in Equations (98) and (99), the substate's conjugate  $\tau_{ij}$  reduces to ( $\tau_{ij} = \frac{\sigma_{ij}}{\rho}$ ). Choosing temperature and Cauchy's strain tensor as state variables, the free energy  $\psi(\eta, \epsilon_{ij}^e)$  can be expressed as,

$$\psi(\theta, \epsilon_{ij}^e) = \frac{\lambda}{2} \epsilon_{kk}^e{}^2 + \mu \epsilon_{ij}^e \epsilon_{ij}^e - 3K \alpha_v \theta_0 \epsilon_{kk}^e \theta - \frac{c_\epsilon}{2\theta_0} \theta^2, \quad (\text{Thermoelasticity}) \quad (100)$$

and its incremental form is

$$d\psi = \lambda \epsilon_{kk}^e d\epsilon_{kk}^e + 2\mu \epsilon_{ij}^e d\epsilon_{ij}^e - 3K \alpha_v \theta_0 (\epsilon_{kk}^e d\theta + \theta d\epsilon_{kk}^e) - \frac{c_\epsilon}{\theta_0} d\theta, \quad (\text{Incremental}) \quad (101)$$

Note that, Equation (100) is obtained by expanding the free energy into the Taylor series in the vicinity of the natural state of strain and temperature retaining only up to second order terms (see Nowacki [12] for full details). Further, substituting the free energy for thermoelastic medium in Equation (100) into Equation (87), then Equation (87) becomes equal to

$$\eta \equiv -\left(\frac{\partial \psi}{\partial \theta}\right)_{\alpha} = 3K\alpha_v\theta_0\epsilon_{kk}^e + \frac{c_\epsilon}{\theta_0}\theta, \quad (\text{Thermoelasticity}) \quad (102)$$

$$\frac{\sigma_{ij}}{\rho} \equiv \left(\frac{\partial \psi}{\partial \epsilon_{ij}^e}\right)_{\theta} = \lambda\delta_{ij}\epsilon_{kk}^e + 2\mu\epsilon_{ij}^e - 3K\alpha_v\theta_0\delta_{ij}\theta, \quad (\text{Thermoelasticity}). \quad (103)$$

and their incremental forms are

$$d\eta = 3K\alpha_v\theta_0d\epsilon_{kk}^e + \frac{c_\epsilon}{\theta_0}d\theta, \quad (\text{Incremental}) \quad (104)$$

$$\frac{1}{\rho}d\sigma_{ij} = \lambda\delta_{ij}d\epsilon_{kk}^e + 2\mu d\epsilon_{ij}^e - 3K\alpha_v\theta_0\delta_{ij}d\theta, \quad (\text{Incremental}). \quad (105)$$

Note that, the free energy and the relations that follow from it for a thermoelastic system characterize the thermostatic state which is a necessary state that a non-equilibrium thermodynamic process is built on and the basis of the development of the thermodynamic model of failure. A clearer picture on how they play a role in the thermodynamic model of failure will be shown later as the failure model is discussed in detail.

Third, the **enthalpy**  $h$  is also a thermodynamic potential which is defined as the portion of the internal energy that can be released as heat when the thermodynamic tensions are held constant, that is

$$h(\eta, \tau) = u - \tau_i\alpha_i. \quad (106)$$

Based on the definition of the enthalpy (see Malvern [6], chapter 5), temperature and substate variables are given as

$$\theta \equiv \left( \frac{\partial h}{\partial \eta} \right)_{\tau}, \quad \alpha_i \equiv \left( \frac{\partial h}{\partial \tau_i} \right)_{\eta}, \quad i = 1, 2, \dots, n. \quad (107)$$

That is, Equation (107) gives a mathematical definition for the entropy  $\eta$  and the thermodynamic tensions  $\tau_i$  in term of the enthalpy. Using the enthalpy definition in Equation (106), the Gibbs relation (Equation (67)) (see Malvern [6], chapter 5) reduces to

$$dh = \theta d\eta + \alpha_i d\tau_i. \quad (108)$$

Note that in the definition of enthalpy, the independent variables used are the entropy  $\eta$  and the thermodynamic tensions  $\tau_i$ . The enthalpy defined in Equation (106), is different from Gibbs definition which is the so-called free enthalpy  $g$  or Gibbs function (see Malvern [6], chapter 5). The free enthalpy  $g$  is defined as

$$g(\theta, \tau) = h - \eta\theta = u - \tau_i \alpha_i - \eta\theta, \quad (109)$$

and it is the enthalpy energy  $h$  without the internal energy due to heat transfe (i.e.  $\eta\theta$ ). Also, the entropy and substate variables can be written as

$$\eta \equiv \left( \frac{\partial g}{\partial \theta} \right)_{\tau}, \quad \alpha_i \equiv \left( \frac{\partial g}{\partial \tau_i} \right)_{\eta}, \quad i = 1, 2, \dots, n, \quad (110)$$

based on the free enthalpy definition. Further, using the free enthalpy definition in Equation (109), the Gibbs relation (Equation (67)) reduces to

$$dg = -\eta d\theta - \alpha_i d\tau_i. \quad (111)$$

Note that in the definition of free enthalpy, the state variables used are temperature  $\theta$  and the thermodynamic tensions  $\tau_i$ .

The stress and strain tensors for an isotropic and homogenous thermoelasticity continuum are linear elastic stress and strain tensors. If an incremental approach is used to solve the problem, then infinitesimal strain-displacement assumption can be used even if large displacements exist in the problem. That is, both the Green and Eulerian strain tensors reduce into Cauchy's strain tensor. Also, the second Piola-Kirchhoff stress tensor and the Eulerian stress tensors reduce to Cauchy's stress tensor. Thus, in the up-dated Lagrangian approach the stress and strain tensors are the incremental Cauchy's stress tensor  $d\sigma_{ij}$  and the incremental Cauchy's strain tensor  $d\epsilon_{ij}^e$ . Considering the thermoelasticity for an isotropic homogenous medium where the state variables are the absolute temperature  $\theta$ , and the thermodynamic tension  $\tau_{ij}$  equal to the stress tensor  $\frac{\sigma_{ij}}{\rho}$ , where its conjugate  $\alpha_{ij}$  becomes equal to Cauchy's strain tensor  $\epsilon_{ij}^e$ , based on Equation (110), then, the free enthalpy  $g$  can be expressed as,

$$g(\theta, \sigma_{ij}) = \left(\frac{2\mu - 3K}{36\mu K}\right)\sigma_{kk}^2 + \frac{1}{4\mu}\sigma_{ij}\sigma_{ij} + \frac{1}{3}\alpha_v\sigma_{kk}\theta + \frac{c_\sigma}{\theta_0}\theta, \quad (\text{Thermoelasticity}) \quad (112)$$

and its incremental form is

$$dg = \left(\frac{2\mu - 3K}{18\mu K}\right)\sigma_{kk}d\sigma_{kk} + \frac{1}{2\mu}\sigma_{ij}d\sigma_{ij} + \frac{1}{3}\alpha_v(\sigma_{kk}d\theta + \theta d\sigma_{kk}) + \frac{c_\sigma}{\theta_0}d\theta, \quad (\text{Incremental}) \quad (113)$$

where  $c_\sigma$  is the specific heat at a constant stress. The thermoelastic free enthalpy  $g$  formulated similar to the thermoelastic internal energy and free energy (see Nowacki [12] for details). Substituting the free enthalpy for thermoelastic medium in Equation (112) into Equation (110), then Equation (110) equals

$$\eta \equiv \left(\frac{\partial g}{\partial \theta}\right)_\tau = \frac{\alpha_v}{3\rho}\sigma_{kk} + \frac{c_\sigma}{\theta_0}\theta, \quad (\text{Thermoelasticity}) \quad (114)$$

$$\epsilon_{ij}^e \equiv \rho \left( \frac{\partial g}{\partial \sigma_{ij}} \right)_\eta = \left( \frac{2\mu - 3K}{18\mu K} \right) \delta_{ij} \sigma_{kk} + \frac{1}{2\mu} \sigma_{ij} + \frac{1}{3} \alpha_v \delta_{ij} \theta . \quad (\text{Thermoelasticity}) \quad (115)$$

and their incremental forms are

$$d\eta = \frac{\alpha_v}{3\rho} d\sigma_{kk} + \frac{c_\sigma}{\theta_0} d\theta , \quad (\text{Incremental}) \quad (116)$$

$$d\epsilon_{ij}^e = \left( \frac{2\mu - 3K}{18\mu K} \right) \delta_{ij} d\sigma_{kk} + \frac{1}{2\mu} d\sigma_{ij} + \frac{1}{3} \alpha_v \delta_{ij} d\theta , \quad (\text{Incremental}) . \quad (117)$$

Note that, the enthalpy and the relations that follow from it for a thermoelastic system characterize the thermostatic state which the thermodynamic process consists of (i.e. a non-equilibrium thermodynamic process is assumed as a transition from one thermostatic state to the other). This will become evident as the thermodynamic model of failure is discussed.

#### IV. Thermodynamic Process

A thermodynamic system is one in which the system's energy both internal energy and energy exchanged through the exterior by means of heat and work evolves in time from one state to another state. This process of thermodynamics could be for a reversible or irreversible process. In a reversible process, the thermodynamic system is characterized by state variables at a moment where thermodynamic equilibrium exists and energy balance is satisfied (i.e. equilibrium is the state where the system does balance the internal and external elements acting on it through an equality relation) and the principles governing reversible thermodynamic processes are established through the thermostatic or thermodynamic equilibrium laws. These laws have been discussed in the previous sections, and they are referred to as laws in the state of equilibrium where the notions of

temperature, entropy,... etc. are well defined. However, for an irreversible thermodynamic process, the process does not have an equilibrium state as in the thermostatic system as it evolve in time. In other words, an irreversible thermodynamic process is the study of a phenomena outside a state of equilibrium, but in the vicinity of an equilibrium state and not far from it. But the principles governing non-equilibrium or an irreversible thermodynamic process are associated with the thermostatic laws of a reversible thermodynamic process, and the thermostatic laws are the bases of the non-equilibrium laws. The notion of thermodynamic quantities such as temperature and entropy are well-defined in thermodynamic equilibrium and will be extended to model non-equilibrium as it evolve in time. This is of importance, because the failure in a continuum is characterized by non-equilibrium or an irreversible thermodynamic process, and it is the core of our study.

Hence, the theory development of an irreversible thermodynamic system depends, in part, on the thermostatic theory, where an irreversible thermodynamic system is conceived as a transition from one state of equilibrium, in thermostatic sense, to another. The concept of transition from one state of equilibrium to another in the analysis of irreversible thermodynamic system allows for the analyses of irreversible thermodynamic processes to be carried out in an incremental fashion. That is, for a thermodynamic process the governing equations representing a thermostatic state, where the thermodynamic quantities such as temperature, entropy, strain, stress, thermodynamic potentials...etc. are well defined, are solved by incrementing the state variables through time. Although, both the state variables and time are incremented, the time rate is the main driver of the incremental process. That is, as the time is being incremented, the state variables are also incremented

to satisfy the thermostatic state (i.e. thermodynamic equilibrium) through the rate relations. Note that, even though for a reversible thermodynamic process the governing equation are computed by an incremental technique. For example, the Hamiltonian principle (i.e. the variational form of the equation of motion) is used to solve the problem in an incremental approach for a structural dynamic problem. The Hamiltonian principle states

$$\int_{t_1}^{t_2} (\delta T + \delta \Pi) dt = 0 , \quad (118)$$

where the time integration is between an initial time  $t_1$  and final time  $t_2$ ,  $\delta T$  is the variation of the kinetic energy and  $\delta \Pi$  is the variation of the potential energy. Manipulating Equation (118) and using the finite element as a numerical solution (see Bath [13]) leads to a finite element governing equation which is

$$[M]\{\ddot{q}\} + [C]\{\dot{q}\} + [K]\{q\} = \{F\} , \quad (119)$$

where  $[M]$  is the mass matrix,  $[C]$  is the damping matrix,  $[K]$  is the stiffness matrix,  $\{F\}$  is the force vector,  $\{q\}$  is the degree of freedom, and  $\{\dot{q}\}$  and  $\{\ddot{q}\}$  are the velocity and acceleration, respectively. Equation (119) is time dependent finite element governing equation which can be solved in an incremental approach in time using finite difference technique. But, for an irreversible thermodynamic process, the governing equation does not represent quantities that are perfect differential compared to the perfect differential quantities for a reversible thermodynamic process. Hence, the irreversible thermodynamic process is conceived as a transition from one state of equilibrium to another, and the thermostatic equations in its time rate form is used to solve the governing equations. For example, the time rate of Equation (114) is

$$\dot{\eta} = \frac{\alpha_v}{3\rho} \dot{\sigma}_{kk} + \frac{c_\sigma}{\theta_0} \dot{\theta} , \quad (120)$$

which is used in combination with the incremental governing equation to solve the problem.

The idea of basing the development of non-equilibrium or irreversible thermodynamic process on thermostatic principles has two representations which mainly differ by their inclusion of the thermostatic process in the formulation of non-equilibrium process. The two main representations are the **Axiomatic** representation, and the **thermodynamics with internal variables** representations. Both representations will be discussed for comparison, but the second will be used in developing the thermodynamic model of failure. Since, the latter has the advantage of representing materials that exhibit time or rate dependent phenomena, such as viscoplastic.

The **Axiomatic** or axiom of local state representation (see Maugin [7], appendix 1) is based on the hypothesis that a material particle in motion should be in equilibrium at practically any moment. The response times which allow the thermostatic system to recover a new state of thermostatic equilibrium must be short, compared with the characteristic duration of the kinematics and dynamic evolution of the medium. In other words, as the thermodynamic process evolves in time, the thermostatic principles must also be satisfied based on the fact that the thermodynamic process transits from one state of thermostatic to another.

On the other hand, the **thermodynamics with internal variables** representation (see Maugin

[7], appendix 1) provides a new characterization of the continuous media in order to define the thermodynamic state of a system. It introduces, in addition to the usual observable state variables, a certain number of internal variables  $\gamma$  to describe the internal structure. These internal variables represent hidden (i.e. implicitly measurable and not controllable internal variables) phenomena, such as plastic deformation due to dislocation movement, i.e. slip of the crystallographic planes in a metal, to the twinning or coupling of crystals, to the slip of the grain boundaries, to a phase transition induced by strain,... etc. In this case, the internal variables  $\gamma$  is characteristic of a local structure rearrangement. Depending on the nature of the problem, these internal variables can represent the material dependent on the rate of loading such as strain or stress rate, such as viscoelastic and elastoplastic material, or characterize failure and its growth in a continuum. Hence, the dependent variables become functions of the state variables and the internal variables. For illustration purposes, consider the dependent variables to be the stress tensor  $\hat{\sigma}_{ij}$ , then each component of the stress tensor become functions of the state variables  $\alpha_{ij}$  and the internal variables  $\gamma_i$ , and can be expressed as

$$\hat{\sigma}_{ij} = \tilde{\sigma}_{ij}(\alpha_{ij}, \gamma_i) \quad \text{Constitutive equations or State Laws ,} \quad (121)$$

$$\dot{\gamma}_i = \varphi_i(\alpha_{ij}, \gamma_i) + \mathfrak{S}_i(\alpha_{ij}, \gamma_i)\dot{\alpha}_{ij} \quad \text{Evolution Laws .} \quad (122)$$

The evolution laws stated in Equation (122) is the time rate equation that govern the internal variables, and it is shown in a general form in Equation (122) where the rate of change of the internal variables are linearly related to the rate of change of the state variables. For the case where  $\varphi$  might be identically zero ( $\varphi = \mathbf{0}$ ), then the instantaneous variations in the state variables  $\alpha_{ij}$  does not cause instantaneous variations in the internal variables  $\gamma_i$ . To illustrate the evolution laws, the continuous model of slip in viscoplasticity for metal (see Maugin [7], appendix 1) is considered as an example. For the continuous model of slip in viscoplastic metal, the internal variables  $\gamma_i$  are the

slip in the  $i$ th simple slip system of the crystal, and it is defined in term of the flow potential  $D^*$  which exists for the system of the crystal and used to define the plastic strain rate  $\dot{\epsilon}^p$  to be normal to the constant flow potential  $D^*$  in the space of stresses as

$$\dot{\epsilon}^p = \frac{\partial D^*}{\partial \sigma} , \quad (123)$$

where  $\dot{\epsilon}^p$  is the rate of plastic strain and  $\sigma$  is the stress tensor. The evolution laws for the continuous model of slip in viscoplasticity for metal is

$$\dot{\gamma}_i = \tilde{\gamma}_i(\theta, \tau_i, \gamma_i) = \frac{\partial D^*}{\partial \zeta_i} , \quad (124)$$

where the internal variable  $\gamma_i$  is the slip in the  $i$ th simple slip system of the crystal, and  $\zeta_i$  are the internal variables conjugates (i.e. the shear stresses related to the  $i$ th simple slip system of the crystal), and it is equal to

$$\zeta_i = \frac{\partial u^*}{\partial \gamma_i} , \quad (125)$$

where  $u^*$  is the complementary internal energy. Furthermore, the thermostatic is formulated including the internal variables. For example, the Gibbs relation (Equation (88)) with internal variables becomes

$$d\psi = -\eta d\theta + \tau_i d\alpha_i - \zeta_i d\gamma_i . \quad (126)$$

where

$$\eta \equiv -\left(\frac{\partial \psi}{\partial \theta}\right)_{\alpha, \gamma_i} , \quad \tau_i \equiv \left(\frac{\partial \psi}{\partial \alpha_i}\right)_{\theta, \gamma_i} , \quad \zeta_i \equiv \left(\frac{\partial \psi}{\partial \gamma_i}\right)_{\alpha, \theta} , \quad i = 1, 2, \dots, n , \quad (127)$$

are relations that govern a thermostatic state.

But, how does the thermostatic laws enter into the picture. The *argument* is as follows: Consider the dependent variable, stress  $\hat{\sigma}_{ij}$  in this case, and suppose in theory, if not in practice, that the internal variables may well keep a prescribed value by the imposition of the appropriate stress  $\hat{\sigma}_{ij}$ , the system then will tend towards a state of thermostatic (thermodynamic equilibrium), characterized by the stress and the state variables which are in this case the strain and temperature. Then suppose that different states of equilibrium are possible for the same values of internal variables, specified above. Then, the neighboring states are connected by the laws of ordinary thermoelasticity, which are established earlier.

These thermostatic principles, i.e. thermoelasticity, that non-equilibrium or irreversible thermodynamic processes are based on, are summarized for an isotropic homogenous medium. The substate variable  $\alpha_{ij}$  is taken equal to Cauchy's strain tensor  $\epsilon_{ij}^e$  and its conjugate  $\tau_{ij}$  become the stress tensor  $\frac{\sigma_{ij}}{\rho}$ , where  $T_{ij}$  is the Cauchy's stress tensor. The ordinary thermoelasticity equations are summarized, and they are:

- The internal energy, Equation (80), free energy, Equation (100), and free enthalpy, Equation (112), are

$$u(\eta, \epsilon_{ij}^e) = \frac{\lambda}{2} \epsilon_{kk}^e \epsilon_{nn}^e + \mu \epsilon_{ij}^e \epsilon_{ij}^e - \frac{K \alpha_v \theta_0}{c_\epsilon} \epsilon_{kk}^e \eta + \theta_0 \eta + \frac{\theta_0}{2c_\epsilon} \eta^2, \quad (80)$$

$$\psi(\theta, \epsilon_{ij}^e) = \frac{\lambda}{2} \epsilon_{kk}^e \epsilon_{nn}^e + \mu \epsilon_{ij}^e \epsilon_{ij}^e - 3K \alpha_v \theta_0 \epsilon_{kk}^e \theta - \frac{c_\epsilon}{2\theta_0} \theta^2, \quad (100)$$

$$g(\theta, \sigma_{ij}) = \left(\frac{2\mu - 3K}{36\mu K}\right)\sigma_{kk}\sigma_{nn} + \frac{1}{4\mu}\sigma_{ij}\sigma_{ij} + \frac{1}{3}\alpha_v\sigma_{kk}\theta, \quad (112)$$

- The absolute temperature, Equation (82), is

$$\theta \equiv \left(\frac{\partial u}{\partial \eta}\right)_\alpha = -\frac{K\alpha_v\theta_0}{c_\epsilon}\epsilon_{kk}^e + \theta_0 + \frac{\theta_0}{c_\epsilon}\eta, \quad (82)$$

- The entropy, in term of the free energy, Equation (102), and in term of the free enthalpy, Equation (114), are

$$\eta \equiv -\left(\frac{\partial \psi}{\partial \theta}\right)_\alpha = 3K\alpha_v\theta_0\delta_{ij}\epsilon_{kk}^e + \frac{c_\epsilon}{\theta_0}\eta, \quad (102)$$

$$\eta \equiv \left(\frac{\partial g}{\partial \theta}\right)_\tau = \frac{c_\epsilon}{\theta_0}(\theta - \theta_0) + \frac{\alpha_v}{\rho}\sigma_{kk}, \quad (114)$$

- The strain tensor (i.e. Cauchy's strain tensor), Equation (115), is

$$\epsilon_{ij}^e \equiv \rho \left(\frac{\partial g}{\partial \sigma_{ij}}\right)_\eta = \left(\frac{2\mu - 3K}{18\mu K}\right)\delta_{ij}\sigma_{kk} + \frac{1}{2\mu}\sigma_{ij} + \frac{1}{3}\alpha_v\delta_{ij}\theta, \quad (115)$$

- The stress tensor (i.e. Cauchy's stress tensor), in term of the internal energy, Equation (83), and in term of the free energy, Equation (103), are

$$\frac{\sigma_{ij}}{\rho} \equiv \left(\frac{\partial u}{\partial \epsilon_{ij}^e}\right)_\eta = \lambda\delta_{ij}\epsilon_{kk}^e + 2\mu\epsilon_{ij}^e - \frac{K\alpha_v\theta_0}{c_\epsilon}\delta_{ij}\eta, \quad (83)$$

$$\frac{\sigma_{ij}}{\rho} \equiv \left(\frac{\partial \psi}{\partial \epsilon_{ij}^e}\right)_\theta = \lambda\delta_{ij}\epsilon_{kk}^e + 2\mu\epsilon_{ij}^e - 3K\alpha_v\theta_0\delta_{ij}\theta, \quad (103)$$

Note that, it was mentioned earlier that non-equilibrium thermodynamic process translate from a thermoelastic state to another which allow for solving the process in an incremental approach. In this case the thermoelastic equations becomes part of an incremental process and they are written in a time rate form. For example, consider a linear elastic continuum for illustration, the Hooke's laws are

$$\sigma_{11} = \lambda \epsilon_{kk} + 2\mu \epsilon_{11} , \quad (128)$$

$$\sigma_{22} = \lambda \epsilon_{kk} + 2\mu \epsilon_{22} , \quad (129)$$

$$\sigma_{33} = \lambda \epsilon_{kk} + 2\mu \epsilon_{33} , \quad (130)$$

$$\sigma_{12} = 2\mu \epsilon_{12} , \quad (131)$$

$$\sigma_{13} = 2\mu \epsilon_{13} , \quad (132)$$

$$\sigma_{23} = 2\mu \epsilon_{23} , \quad (133)$$

and taking the time derivative, their time rate are

$$\dot{\sigma}_{11} = \lambda \dot{\epsilon}_{kk} + 2\mu \dot{\epsilon}_{11} , \quad (134)$$

$$\dot{\sigma}_{22} = \lambda \dot{\epsilon}_{kk} + 2\mu \dot{\epsilon}_{22} , \quad (135)$$

$$\dot{\sigma}_{33} = \lambda \dot{\epsilon}_{kk} + 2\mu \dot{\epsilon}_{33} , \quad (136)$$

$$\dot{\sigma}_{12} = 2\mu \dot{\epsilon}_{12} , \quad (137)$$

$$\dot{\sigma}_{13} = 2\mu \dot{\epsilon}_{13} , \quad (138)$$

$$\dot{\sigma}_{23} = 2\mu \dot{\epsilon}_{23} , \quad (139)$$

where  $\lambda$  and  $\mu$  are Lamé constants, and their incremental form reduces to

$$d\sigma_{11} = \lambda d\epsilon_{kk} + 2\mu d\epsilon_{11} , \quad (140)$$

$$d\sigma_{22} = \lambda d\epsilon_{kk} + 2\mu d\epsilon_{22} , \quad (141)$$

$$d\sigma_{33} = \lambda d\epsilon_{kk} + 2\mu d\epsilon_{33} , \quad (142)$$

$$d\sigma_{12} = 2\mu d\epsilon_{12} , \quad (143)$$

$$d\sigma_{13} = 2\mu d\epsilon_{13} , \quad (144)$$

$$d\sigma_{23} = 2\mu d\epsilon_{23} , \quad (145)$$

where the stress tensor, for example, at increment  $(n + 1)$  is

$$\sigma^{(n+1)} = \sigma^{(n)} + d\sigma^{(n)} , \quad (146)$$

where the superscribe values between the parenthesis indicate the increment number.

Note that, by eliminating the internal variables  $\gamma_i$  from the constitutive or state laws (Equations (121)) using the evolution laws (Equation (122)) leads to a time-functional law for the stress  $\sigma_{ij}$ . This shows that the problem is placed in a time-domain. Hence, this representation becomes advantages for modeling materials that exhibit time or rate dependent phenomena, such as viscoplastic, elastoplastic, and viscoplastic, compared with the axiomatic representation. Furthermore, the **thermodynamics with internal variables** representations provides a new characterization of a continuous media, which in order to define the thermodynamic state of a system, introduces, in addition to the usual observable state variables, a certain number of internal variables to describe

the internal structure. These internal variables represent hidden mechanisms, such as micromechanics damage which is not explicitly measurable but implicitly and not controllable. These reasons are behind the use of the thermodynamics with internal variables representation in developing a thermodynamic model of failure.

## 2.2 Thermodynamic Model of Failure

Nonlinear response and failure initiation in a medium within a thermodynamic system are associated with an irreversible process. That is, part of the energy supplied through external forces and heat dissipation can not be recovered, which causes a change in the atomic-structure and its bond strength. Thus, for a continuum, as the work and heat input act on the system raising its internal energy, the atomic-structure of the material experiences frictional dissipation in addition to certain complex phenomena that happen at the microscopic level (e.g. such as plastic deformation, cavity initiation, and damage growth). The thermodynamic model of failure presented by Kiselev and Yumashev [5] is based on energy dissipation and it models an elastoplastic material. The mathematical derivation of the state equations for this thermodynamic model will be presented and discussed next.

For this model, the substate variables used to characterize the thermodynamic failure model are the elastic strain  $\epsilon_{ij}^e$ , plastic strain  $\epsilon_{ij}^p$ , and an internal variable  $\gamma$  associated with the damage dissipation in the continuum. Note that, the internal variable  $\gamma$  describes the initiation and growth of damage for the material during deformation. The internal variable  $\gamma$  is called structural damage parameter which is assumed that it vary from zero for undamaged structure, and become equal to one for totally damaged structure.

It is important to note that certain assumptions are made by Kiselev and Yumashev [5] which are the following. First, the strain tensor is written in two parts the elastic strain  $\epsilon_{ij}^e$  and the plastic strain  $\epsilon_{ij}^p$ , that is

$$\epsilon_{ij} = \epsilon_{ij}^e + \epsilon_{ij}^p . \quad (147)$$

Forming the time rate of Equation (148) by taking its derivative with respect to time, the incremental form of the total strain  $\epsilon_{ij}$  reduces to

$$d\epsilon_{ij} = d\epsilon_{ij}^e + d\epsilon_{ij}^p . \quad (148)$$

Second, the elastic strain  $\epsilon_{ij}^e$  is a linear elastic strain, i.e. infinitesimal strain where the strain used is the Cauchy strain tensor  $\epsilon_{ij}^e$ , and the corresponding stress is the Cauchy's stress tensor  $\sigma_{ij}$ . In other words, since the incremental approach is chosen to solve the problem, then the assumption of infinitesimal stress-strain response due to infinitesimal strain-displacement relations can be used even though large displacements exist (i.e. effects of large displacements on the behavior of the problem can be captured using an incremental approach even though an infinitesimal stress-strain response). Also, the incremental approach is a necessary one to solve the inelastic behavior such as the plasticity which is a nonconservative rate dependent process. Third, the model's governing equations are formulated using Lagrangian representation where the updated Lagrangian approach is chosen to solve them numerically.

The mathematical derivation of the thermodynamic model of failure consist of the conservation's laws, the first and second law of thermodynamics, and the state laws or the constitutive laws of the continuum, and they will be presented in the same order. The conservation laws where Cauchy stress tensor is used instead of the second Piola-Kirchhoff stress tensor  $P_{IJ}$  under the assumption of infinitesimal strain are the following. The conservation of mass given in Equation (22) reduces to

$$\dot{\rho} = 0 . \quad (149)$$

The conservation of linear momentum given in Equation (28) becomes

$$\sigma_{ij,j} + \rho b_i = \rho \dot{v}_i . \quad (150)$$

The conservation of angular momentum Equation (33) is given as

$$\sigma_{ij} = \sigma_{ji} , \quad (151)$$

which indicate that the Cauchy stress tensor  $\sigma_{ij}$  is symmetric.

The first law and second law of thermodynamics are as follows. Assuming no heat source  $r_h$  in the continuum and no body forces  $\mathbf{b}$ , the state equations of the first and second law of thermodynamics, Equations (46) and (60), becomes

$$\dot{u} = \frac{\sigma_{ij} \epsilon_{ij}}{\rho} - \frac{q_{i,i}}{\rho} , \quad (152)$$

$$\dot{\eta} \geq -\frac{q_{i,i}}{\theta} + \frac{q_i \theta_{,i}}{\theta^2} , \quad (153)$$

respectively. Using the temperature  $\theta$ , the elastic strain  $\epsilon_{ij}^e$ , the plastic strain  $\epsilon_{ij}^p$ , and the structural damage parameter  $\gamma$ , as the independent variables for the free energy  $\psi(\theta, \epsilon_{ij}^e, \epsilon_{ij}^p, \gamma)$  shown in

Equation (86), then its time derivative is

$$\dot{\psi} = \frac{\partial \psi}{\partial \epsilon_{ij}^e} \dot{\epsilon}_{ij}^e + \frac{\partial \psi}{\partial \epsilon_{ij}^p} \dot{\epsilon}_{ij}^p + \frac{\partial \psi}{\partial \theta} \dot{\theta} + \frac{\partial \psi}{\partial \gamma} \dot{\gamma}. \quad (154)$$

The second law of thermodynamic can also be rewritten in terms of the free energy. That is, using the definition of the free energy in Equation (86) to eliminate entropy from the second law Equation (153), it reduces to

$$\frac{\partial}{\partial t} \left( \frac{u - \psi}{\theta} \right) \geq -\frac{q_{i,i}}{\theta} + \frac{q_i \theta_{,i}}{\theta^2}. \quad (155)$$

Then perform the time derivative on the left-hand side of Equation (155) leads to

$$\frac{1}{\theta^2} (\theta \dot{u} + \psi \dot{\theta} - u \dot{\theta} - \theta \dot{\psi}) \geq -\frac{q_{i,i}}{\theta} + \frac{q_i \theta_{,i}}{\theta^2}, \quad (156)$$

and rearranging Equation (156) one obtains

$$\frac{1}{\theta} (\dot{u} - \dot{\psi}) + \frac{\dot{\theta}}{\theta^2} (\psi - u) \geq -\frac{q_{i,i}}{\theta} + \frac{q_i \theta_{,i}}{\theta^2}. \quad (157)$$

Then, using the first law (Equation (152)) to replace  $\dot{u}$  in the first term of the left hand side of Equation (157), substituting the free energy definition, Equation (86), in the second term, and rearranging, Equation (157) reduces to

$$\frac{\sigma_{ij} \dot{\epsilon}_{ij}^e}{\rho} - \dot{\psi} - \eta \dot{\theta} - \frac{q_i \theta_{,i}}{\rho \theta} \geq 0. \quad (158)$$

In addition, using the time derivative of the free energy (Equation (154)) and rearrange, Equation (158) reduces to

$$\left( \frac{\sigma_{ij}}{\rho} - \frac{\partial \psi}{\partial \epsilon_{ij}^e} \right) \dot{\epsilon}_{ij}^e - \left( \frac{\partial \psi}{\partial \theta} + \eta \right) \dot{\theta} + \frac{1}{\rho} \sigma_{ij} \dot{\epsilon}_{ij}^p - \frac{\partial \psi}{\partial \epsilon_{ij}^p} \dot{\epsilon}_{ij}^p - \frac{\partial \psi}{\partial \gamma} \dot{\gamma} - \frac{q_i \theta_{,i}}{\rho \theta} \eta \dot{\theta} - \frac{q_i \theta_{,i}}{\rho \theta} \geq 0. \quad (159)$$

That is the dissipation function  $d$  becomes equal to

$$d = \left( \frac{\sigma_{ij}}{\rho} - \frac{\partial \psi}{\partial \epsilon_{ij}^e} \right) \dot{\epsilon}_{ij}^e - \left( \frac{\partial \psi}{\partial \theta} + \eta \right) \dot{\theta} + \left( \frac{\sigma_{ij}}{\rho} - \frac{\partial \psi}{\partial \epsilon_{ij}^p} \right) \dot{\epsilon}_{ij}^p - \frac{\partial \psi}{\partial \gamma} \dot{\gamma} - \frac{q_i \theta_{,i}}{\theta}, \quad (160)$$

and Equation (159) can be written as,

$$d \geq 0 \quad (161)$$

This dissipation function  $d$  will be discussed subsequently. From Equations (102) and (103), the first and second parenthesis terms in the dissipation function  $d$  (Equation (160)) vanish, and the dissipation function  $d$  (Equation (160)) becomes

$$d = \left( \frac{\sigma_{ij}}{\rho} - \frac{\partial \psi}{\partial \epsilon_{ij}^p} \right) \dot{\epsilon}_{ij}^p - \frac{\partial \psi}{\partial \gamma} \dot{\gamma} - \frac{q_i \theta_{,i}}{\theta} , \quad (162)$$

The three terms in the dissipation function  $d$  are called the mechanical dissipation  $d_m$ , the dissipation of continual failure  $d_f$ , and the thermal dissipation  $d_\theta$ , respectively, and they are defined as

$$d_m = t_{ij} \dot{\epsilon}_{ij}^p = \left( \frac{\sigma_{ij}}{\rho} - \frac{\partial \psi}{\partial \epsilon_{ij}^p} \right) \dot{\epsilon}_{ij}^p , \quad d_f = -\frac{\partial \psi}{\partial \gamma} \dot{\gamma} , \quad d_\theta = \frac{q_i \theta_{,i}}{\theta} , \quad (163)$$

where  $t_{ij}$  is the active stress tensor and defined as

$$t_{ij} = \frac{\sigma_{ij}}{\rho} - \frac{\partial \psi}{\partial \epsilon_{ij}^p} , \quad (164)$$

where  $\frac{\partial \psi}{\partial \epsilon_{ij}^p}$  is the plastic stress threshold which depends upon the plastic strain  $\epsilon_{ij}^p$  and  $t$  is the portion of the stress beyond the plastic stress threshold where the material plastically deformed. Note that, the mechanical dissipation  $d_m$  represents the dissipation due to the plastic flow, the dissipation of continual failure  $d_f$  represents the dissipation due to the damage mechanism the continuum suffers, and the thermal dissipation  $d_\theta$  represents the heat energy dissipation occurring from the hotter temperature to the colder temperature. In this failure model, more restriction on the thermodynamic process will be imposed than that imposed by the Clausius-Duhem inequality by introducing the following inequalities,

$$d_m \geq 0 , \quad d_f \geq 0 , \quad d_\theta \geq 0 . \quad (165)$$

That is, the mechanical dissipation  $d_m$ , the dissipation of continual failure  $d_f$ , and the thermal dissipation  $d_\theta$ , must be always positive or zero which mean that these dissipation quantities can be created but can not be destroyed, and they are irreversible similar to the entropy concepts. This assumption insures that all three dissipations, i.e. the mechanical dissipation  $d_m$ , the dissipation of continual failure  $d_f$ , and the thermal dissipation  $d_\theta$ , always causes damage in the structure accumulatively and they do not cancel each other effect (i.e. if any of the three dissipation is negative then the dissipation function  $d$  is reduced).

Further, to eliminate the internal energy in term of the free energy, the free energy (Equation (86)) and its time derivative (Equation (154)) are substituted into the first law of thermodynamic (Equation (152)), also substitute the thermoelastic Equations (102) and (83) to simplify terms, the first law of thermodynamic (Equation (152)) can be rewritten as

$$\left(\frac{\sigma_{ij}}{\rho} - \frac{\partial \psi}{\partial \epsilon_{ij}^p}\right) \dot{\epsilon}_{ij}^p - \frac{\partial \psi}{\partial \gamma} \dot{\gamma} - \frac{q_{i,i}}{\rho} - \theta \dot{\eta} = 0, \quad (166)$$

Next, the dissipation of the continual failure  $d_f$  is discussed. The assumption of continual failure  $d_f$  is the rate of energy dissipation and expresses in term of a rate  $\dot{\gamma}$  and thermodynamic tension  $\frac{\partial \psi}{\partial \gamma}$ . For such quantity, it is quite natural to assume, at least close to equilibrium (i.e. thermostatic state), a relation between the rates and the thermodynamic tension (see Prigogine [14], Chapter 4). Such an assumption automatically includes empirical laws such as the Fourier's law for heat transfer in Equations (38) and (39). These linear laws are called phenomenological relations. It is clear

that the existence of such relations is an extra-thermodynamic hypothesis and it is quite conceivable that in some particular cases the relationships between the rate and thermodynamic tension is not linear. However, assuming this linear relation yields an important information concerning the phenomenological coefficients without invoking more complicated (i.e. nonlinear) assumption [14]. Thus, assume that the partial derivative of the free energy  $\psi$  with respect to the structural damage parameter  $\gamma$  is linearly proportional to the time rate of change of the structural damage parameter  $\dot{\gamma}$ , that is

$$-\frac{\partial\psi}{\partial\gamma} = \Upsilon\dot{\gamma} , \quad (167)$$

where  $\Upsilon$  is the phenomenological coefficient of damage and it is a material constant parameter. Thus, substitute Equation (167) into the dissipation of the continual failure  $d_f$  given in Equation (163) produces

$$d_f = -\frac{\partial\psi}{\partial\gamma}\dot{\gamma} = \Upsilon\dot{\gamma}^2 , \quad (168)$$

which shows that the dissipation of the continual failure  $d_f$  becomes quadratic in terms of the time rate of change of the structural damage parameter  $\dot{\gamma}$ . Furthermore, the linear assumption in Equation (167) is in time rate form which can be solved using an incremental approach. Thus, the dissipation of continual failure  $d_f$  can be written in a quadratic form of the structural damage parameter,

$$d_f = -\frac{\partial\psi}{\partial\gamma}\dot{\gamma} \geq 0 , \quad (169)$$

and since ( $d_f \geq 0$ ) then ( $\Upsilon \geq 0$ ).

Furthermore, take the time derivatives of the entropy in the thermoelastic Equation (114) produces

$$\dot{\eta} = \frac{c_\epsilon}{\theta_0} \dot{\theta} + \frac{\alpha_v}{\rho} \dot{\sigma}_{kk} , \quad (170)$$

and substituting it into Equation (166) after using the definition for the dissipation of continual failure  $d_f$  in Equation (168), the first law of thermodynamics, Equation (166), can be written as

$$\rho c_\sigma \dot{\theta} + \frac{\alpha_v}{3} \theta \dot{\sigma}_{kk} = t_{ij} \dot{\epsilon}_{ij}^p + \Upsilon \dot{\gamma}^2 - q_{i,i} . \quad (171)$$

Note that Equation (171) is an energy balance coupling the mechanical and thermal energy. It is also nothing more than the governing equation of a heat transfer in term of the time rate of change of temperature. Using the Fourier's law defined in Equation (39) and using an incremental approach, the temperature is computed based on Equation (171).

Next, the free enthalpy  $g$  for this model is presented as follow. First, since the temperature  $\theta$ , the elastic strain  $\epsilon_{ij}^e$ , the plastic strain  $\epsilon_{ij}^p$ , and the structural damage parameter  $\gamma$ , are the independent variables for the free enthalpy, i.e.  $g(\theta, \sigma_{ij}, \epsilon_{ij}^p, \gamma)$ , then its time derivative is

$$\dot{g} = \frac{\partial g}{\partial \sigma_{ij}} \dot{\sigma}_{ij} + \frac{\partial g}{\partial \epsilon_{ij}^p} \dot{\epsilon}_{ij}^p + \frac{\partial g}{\partial \theta} \dot{\theta} + \frac{\partial g}{\partial \gamma} \dot{\gamma} . \quad (172)$$

Based on Equation (172) and the time derivative of the free energy (Equation (154)) the time derivative of Equation (109), that is the definition of enthalpy  $g$ , becomes

$$\dot{g} = \frac{\partial \psi}{\partial \epsilon_{ij}^e} \dot{\epsilon}_{ij}^e + \frac{\partial \psi}{\partial \epsilon_{ij}^p} \dot{\epsilon}_{ij}^p + \frac{\partial \psi}{\partial \theta} \dot{\theta} + \frac{\partial \psi}{\partial \gamma} \dot{\gamma} - \frac{2}{\rho} \sigma_{ij} \dot{\epsilon}_{ij}^e . \quad (173)$$

Next, substitute the thermoelasticity Equations (102) and (103) into Equations (173) and multiplying the results by the density  $\rho$ , produces

$$\rho \dot{g} = -\epsilon_{ij}^e \dot{\sigma}_{ij} - \rho \eta \dot{\theta} + \rho \frac{\partial \psi}{\partial \epsilon_{ij}^p} \dot{\epsilon}_{ij}^p + \rho \frac{\partial \psi}{\partial \gamma} \dot{\gamma} . \quad (174)$$

Substituting the time derivative of the enthalpy, which is given in Equation (172), into the left hand side of Equation (174), and collect the terms according to the independent variables, Equation (174) reduces to

$$(\epsilon_{ij}^e - \rho \frac{\partial g}{\partial \sigma_{ij}}) \dot{\sigma}_{ij} + \rho (\eta + \frac{\partial g}{\partial \theta}) \dot{\theta} + \rho (\frac{\partial \psi}{\partial \epsilon_{ij}^p} - \frac{\partial g}{\partial \epsilon_{ij}^p}) \dot{\epsilon}_{ij}^p + \rho (\frac{\partial \psi}{\partial \gamma} - \frac{\partial g}{\partial \gamma}) \dot{\gamma} = 0 . \quad (175)$$

Since  $\dot{\sigma}_{ij}$ ,  $\dot{\theta}$ ,  $\dot{\epsilon}_{ij}^p$ , and  $\dot{\gamma}$  are independent variables and Equation (175) must be satisfied for all of their values at all times, then the terms inside the parenthesis in Equation (175) must vanish leading to the following relations,

$$\epsilon_{ij}^e = \rho \frac{\partial g}{\partial \sigma_{ij}} , \quad \eta = -\frac{\partial g}{\partial \theta} , \quad \frac{\partial \psi}{\partial \epsilon_{ij}^p} = \frac{\partial g}{\partial \epsilon_{ij}^p} , \quad \frac{\partial \psi}{\partial \gamma} = \frac{\partial g}{\partial \gamma} . \quad (176)$$

The free enthalpy  $g$  is obtain by integrating Equation (174) with respect to time which produces

$$\rho g = \int \rho \dot{g} dt = \int [-\sigma_{ij} \dot{\epsilon}_{ij}^e - \rho \eta \dot{\theta} + \rho \frac{\partial \psi}{\partial \epsilon_{ij}^p} \dot{\epsilon}_{ij}^p + \rho \frac{\partial \psi}{\partial \gamma} \dot{\gamma}] dt , \quad (177)$$

using the definition of the dissipation of continual failure  $d_f$  in Equation (168) reduces Equation (177) to

$$\rho g = \int \rho \dot{g} dt = \int [-\sigma_{ij} \dot{\epsilon}_{ij}^e - \rho \eta \dot{\theta} + \rho \frac{\partial \psi}{\partial \epsilon_{ij}^p} \dot{\epsilon}_{ij}^p - \rho \Gamma \dot{\gamma}^2] dt , \quad (178)$$

and eliminating elastic strain  $\epsilon_{ij}^e$  and entropy  $\eta$  in term of the stress tensor  $\sigma_{ij}$  and temperature  $\theta$  using the thermoelasticity Equations (115) and (114), respectively, the free enthalpy can be written as

$$-\rho g = \left( \frac{2\mu - 3K}{36\mu K} \right) \sigma_{kk}^2 + \frac{1}{4\mu} \sigma_{ij} \sigma_{ij} + \frac{1}{3} \alpha_v \sigma_{kk} (\theta - \theta_0) - \int \rho \frac{\partial g}{\partial \epsilon_{ij}^p} d\epsilon_{ij}^p + \Upsilon \int_0^\gamma \dot{\gamma} d\gamma + g_0(\theta) , \quad (179)$$

where  $g_0(\theta)$  is the free enthalpy as a function of temperature in the natural state.

Next, the constitutive laws that has been used by Kiselev and Yumashev [5] is discussed. First, the damage mechanics assumes that material properties such as the elastic modulus, shear modulus, ...etc. are less than their undamaged value based on a damage criterion. Thus, Kiselev and Yumashev [5] assumed that as the damage in the material progresses, the bulk modulus, the shear modulus, and Lamé's constants are functions of the damage (i.e.  $\gamma$ ). That is, material constants for an elastic medium are assumed to change linearly with damage, and it is assumed to degrade in the following linear form

$$K(\gamma) = K_0(1 - \gamma) , \quad (180)$$

$$\mu(\gamma) = \mu_0(1 - \gamma) , \quad (181)$$

$$\lambda(\gamma) = \lambda_0(1 - \gamma) , \quad (182)$$

where  $K_0$  is the bulk modulus and  $\mu_0$  and  $\lambda_0$  are Lamé's constants for an undamaged structure which may depend on temperature, pressure and other parameters, Wilkins [15]. This assumption shows that the strength of the linear elastic part of the material is affected by the damage and as the damage grows in the continuum, its elastic strength is softened or reduced based on the above relation.

For the elastoplastic behavior of the material the following constitutive laws are adopted. First,

assuming that the damage affect the mechanical material properties directly as in Equations (180)-(182), then the damage also affect the mechanical stresses which are referred to as the effective stress tensor  $\sigma'_{ij}$  and it is defined as

$$\sigma'_{ij} = \frac{\sigma_{ij}}{(1 - \gamma)} . \quad (183)$$

To illustrate this, for example, consider the Hooke's laws along the 11-directions, that is

$$\sigma_{11} = \lambda \epsilon_{kk} + 2\mu \epsilon_{11} , \quad (184)$$

and using the damaged Lamé' constants in equations (181) and (182) produce

$$\sigma_{11} = \lambda_0(1 - \gamma)\epsilon_{kk} + 2\mu_0(1 - \gamma)\epsilon_{11} , \quad (185)$$

divide by  $(1 - \gamma)$  gives the effective stress tensor  $\sigma'_{11}$  which is

$$\sigma'_{11} = \frac{\sigma_{11}}{(1 - \gamma)} = \lambda_0\epsilon_{kk} + 2\mu_0\epsilon_{11} , \quad (186)$$

Hence, using this definition of the effective stress tensor  $\sigma'_{ij}$ , the deviatoric stress tensor  $S_{ij}$  is defined as

$$\begin{aligned} S_{ij} &= \sigma_{ij} - \frac{1}{3}\sigma_{kk}\delta_{ij} , \\ S'_{ij} &= \frac{S_{ij}}{(1 - \gamma)} . \end{aligned} \quad (187)$$

The deviatoric strain tensor  $e_{ij}$  is defined as

$$e_{ij} = \epsilon_{ij} - \frac{1}{3}\epsilon_{kk}\delta_{ij} . \quad (188)$$

Also, the plastic flow is assumed incompressible, i.e.,

$$\epsilon_{kk}^p = 0 . \quad (189)$$

Based on the stresses being functions of the damage  $\gamma$ , Kiselev and Yumashev [5] used the elastoplastic flow model of Prandtl-Reuss [15, 16]. Prandtl-Reuss elastoplastic flow model states

$$(S'_{ij})^\nabla + \bar{\lambda} S'_{ij} = 2\mu_0 \dot{e}_{ij} , \quad (190)$$

where the symbol  $( )^\nabla$  signifies Jaumann derivative of a tensor which is the time rate of change of stress in the deformed coordinate system after eliminating the rigid body rotation, and it will be discussed subsequently,  $\bar{\lambda}$  is the plasticity proportionality factor which is equal to

$$\bar{\lambda} = 0 , \quad (191)$$

for an elastic region, i.e. the Mises plastic criteria  $S'_{ij} S'_{ij} \leq \frac{2}{3} Y^2$  is satisfied where  $Y$  is the yield stress, and for the plastic region it equal to

$$\bar{\lambda} = 3 \frac{\mu_0}{Y^2} S'_{ij} \dot{e}'_{ij} H(S'_{ij} \dot{e}'_{ij}) , \quad (192)$$

where  $H(x)$  is the Heavyside unit step function which is defined as

$$\begin{aligned} H(x) &= 0 , & \text{if } x \leq 0 , \\ H(x) &= 1.0 , & \text{if } x > 0 . \end{aligned} \quad (193)$$

$$(194)$$

Thus, the Heavyside unit step function  $H$  in Equation (192) is to insure that the plasticity proportionality factor  $\bar{\lambda}$  defined in Equations (192) is incorporated only in the plastic region, otherwise it is zero as given in Equation (191). The Prandtl-Reuss elastoplastic flow rule defined in Equations (190)-(192) states that the rate of stress and strain are related in the plastic region. Note that the

Prandtl-Reuss elastoplastic flow rule is a realistic description of the plastic behavior of metals when anisotropy (e.g. composite) and Bauschinger effects (i.e. the yield stress for tension and compression are different for material in non-virgin state) are of secondary importance.

Furthermore, the constitutive relations (i.e. the flow rules) are formulated as rate (i.e. incremental) laws where the rates of stresses and strain are related rather than the stress being related to the strain as in the Hooke's law. Since the deformation rate is unaffected by the rigid body rotation of the material, the stress rate must also be independent of the rigid body rotation. This is the reason for using the Jaumann stress rate symbol  $(\sigma_{ij})^\nabla$  and it is defined as

$$(\sigma_{ij})^\nabla = \lim_{\Delta t \rightarrow 0} \left[ \frac{\tilde{\sigma}_{ij}(t + \Delta t) - \tilde{\sigma}_{ij}(t)}{\Delta t} \right], \quad (195)$$

where  $\tilde{\sigma}_{ij}$  are the stress components referred to a coordinate system that translate and rotate (i.e. deformed coordinate system) with material point as time evolve from  $t$  to  $t + \Delta t$  which is consistence with solving the problem in an incremental approach (see Figure 7). Thus, first the stresses at the deformed coordinate system are transformed into the undeformed coordinate system at time  $t$  using the cosine of the angles between unit vectors in the deformed and undeformed coordinate system (see Malvern [6], chapter 3 or any strength of material book), that is

$$\tilde{\sigma}_{ik}(t + \Delta t) = \xi_i \xi_k \sigma_{ij}(t + \Delta t) \quad (196)$$

where  $\xi_i$  is the cosine angles between the unit vector of the deformed and undeformed coordinate system and assuming the deformed and undeformed system rotate  $\omega_{12}$  about the normal unit vector,

the cosine angles  $\xi_{li}$  become

$$\begin{aligned}\xi_{11} &= \xi_{22} = \cos(\omega_{12}\Delta t) \simeq 1 , \\ \xi_{21} &= \xi_{12} = \cos\left(\frac{\pi}{2} - \omega_{12}\Delta t\right) = \sin(\omega_{12}\Delta t) \simeq \omega_{12}\Delta t ,\end{aligned}\tag{197}$$

where the rotation  $\omega_{12}$  assumed small which is consistent with the infinitesimal assumptions. The cosine angles relations between the unit vector of the deformed and undeformed coordinate system defined in Equation (197) can be summarized as

$$\xi_{ij} = \delta_{ij} + \omega_{ij}\Delta t ,\tag{198}$$

where  $\omega_{ii}$  (no sum on  $i$ ) are zero ( $\omega_{ii} = 0$ ) that is the unit vectors are free to spin. Substitute Equation (198) into Equation (195) produce

$$(\sigma_{ij})^\nabla = \lim_{\Delta t \rightarrow 0} \left[ \frac{\sigma_{ij}(t + \Delta t) - \sigma_{ij}(t)}{\Delta t} \right] - \omega_{li}\sigma_{lj} - \omega_{kj}\sigma_{ik} ,\tag{199}$$

where the term in the bracket is the derivative  $\frac{D}{Dt}$  and Equation (199) reduce to

$$(\sigma_{ij})^\nabla = \frac{D\sigma_{ij}}{Dt} - \omega_{li}\sigma_{lj} - \omega_{kj}\sigma_{ik} ,\tag{200}$$

In Equation (200), the first term is the rate of change of the stress with respect to coordinate system moving with the particle (i.e. including rigid body rotation) and the second and third terms results from the formulation to eliminate the rigid body rotation of the material. Note that the stresses in Equation (200) are the time rate of the Cauchy stresses (i.e. the incremental Cauchy stresses), and the problem is solved in an incremental process.

Taking account of the strain anisotropy which is associated with the active stress tensor  $t_{ij}$ , then the flow rule and the Mises criteria become

$$(\tau'_{ij})^\nabla + \bar{\lambda}\tau'_{ij} = 2\mu_0\dot{\epsilon}_{ij}, \quad (201)$$

$$\tau'_{ij}\tau'_{ij} \leq \frac{2}{3}, \quad (202)$$

where  $\tau_{ij}$  is the deviatoric active stress defined as

$$\tau_{ij} = S_{ij} - \rho \frac{\partial g}{\partial \epsilon_{ij}^p} = S_{ij} + \Gamma \epsilon_{ij}^p, \quad (203)$$

$$\tau'_{ij} = \frac{\tau_{ij}}{(1-\gamma)}, \quad (204)$$

where  $\Gamma$  is plasticity proportionality factor. Also, Kiselev and Yumashev [5] defined the rate of the damage dissipation parameter  $\gamma$  based on the kinetic equation of the Tuler-Butcher type [17] as

$$\dot{\gamma} = B(\sigma' - \sigma^*)^m H\left(\frac{\sigma'}{3} - \sigma^*\right), \quad (205)$$

where  $H$  is the Heavyside unit step function defined in Equation (193),  $B$  and  $m$  are material parameters,  $\sigma^*$  is the threshold of the hydrostatic stress  $\frac{\sigma'_{kk}}{3}$  after damage initiation, and  $\sigma'$  is the effective hydrostatic stresses (i.e.  $\sigma' = \sigma'_{kk} = \frac{\sigma_{kk}}{(1-\gamma)}$ ) which is obtain by taking the partial derivative of Equation (179) with respect to the stress which gives

$$-\rho \frac{\partial g}{\partial \sigma_{ij}} = \frac{\partial}{\partial \sigma_{ij}} \left[ \left( \frac{2\mu - 3K}{36\mu K} \right) \sigma_{kk}^2 + \frac{1}{4\mu} \sigma_{ij} \sigma_{ij} + \frac{1}{3} \alpha_v \sigma_{kk} (\theta - \theta_0) - \int \rho \frac{\partial g}{\partial \epsilon_{ij}^p} d\epsilon_{ij}^p + \Upsilon \int_0^\gamma \dot{\gamma} d\gamma + g_0(\theta) \right], \quad (206)$$

also the partial derivative of the free enthalpy  $g$  is related to the elastic strain  $\epsilon_{ij}^e$  based on Equation (176) (i.e.  $\epsilon_{ij}^e = \rho \frac{\partial g}{\partial \sigma_{ij}}$ ), thus taking the trace (e.g.  $\text{tr} \sigma_{ij} = \sigma_{kk}$ ) of Equation (206) produces

$$\sigma' = K_0 [\epsilon_{kk} - \alpha_v (\theta - \theta_0) - \frac{\Lambda}{3} \int_0^\gamma \frac{\partial \dot{\gamma}}{\partial \sigma} d\gamma], \quad (207)$$

Note that the Heavyside unit step function  $H$  in Equation (205) shows that damage initiations only occurs if the hydrostatic stress  $\frac{\sigma'}{3}$  is greater than a threshold of the hydrostatic stress  $\sigma^*$ .

Furthermore, for isotropic homogenous material the yield function is computed based on the second invariant  $J_2$  of the stress deviator (i.e.  $J_2 = \frac{1}{2}S_{ij}S_{ij}$ ) such as the Mises yield function which state that the yield function is equal to the second invariant  $J_2$  of the stress deviator

$$J_2 - Y^2 = \frac{1}{2}S_{ij}S_{ij} - Y^2 = 0 , \quad (208)$$

That is the Mises yield function depend on the stress deviators  $S_{ij}$  only. However, in an impact problem, there are parameter other than the stress deviators that the yield function depend on. Thus, Kiselev and Yumashev [5] assume that the yield strength  $Y$ , the undamaged shear modulus  $\mu_0$ , and the undamaged bulk modulus  $K_0$  depends on temperature, pressure, and material parameters, based on Steinberg-Guinan relation [18] for the yield strength. That is the yield strength  $Y$  is nonlinearly dependent on the temperature, pressure, and material parameters as well as the relative volume  $V_r$  and the equivalent plastic strain and it is defined as

$$\epsilon_u^p = \left( \frac{2}{3} \epsilon_{ij}^p \epsilon_{ij}^p \right)^{\frac{1}{2}} . \quad (209)$$

The yield strength function  $Y$  for an impact problem is a nonlinear function [18] which is given as

$$Y = Y_0(1 + b_1 \epsilon_u^p)^n [1 - b_2 \sigma V_r^{\frac{1}{3}} - b_3(\theta - \theta_0)] , \quad (210)$$

with the conditions

$$Y_0(1 + b_1 \epsilon_u^p)^n \leq Y_{max} , \quad (211)$$

$$Y_0 = 0 \quad \text{for } \theta > \theta_m , \quad \text{where } \theta_m = \theta_{m0} V_r^{\frac{2}{3}} e^{2\zeta_0(1-V_r)} , \quad (212)$$

where  $\theta_m$  is the melting temperature which is material dependent and exponentially function of the relative volume,  $\theta_0$  is the temperature at the reference state which is undamage state,  $Y_0$  is the undamaged yield strength of the material and it is a lower bound (i.e.  $\theta = \theta_0$  and  $\epsilon_u^p = \sigma = 0$  then  $Y = Y_0$ ), and  $n, b_1, b_2, b_3, \theta_{mo}$ , and  $\zeta_0$  are material constants. In this constitutive model it provides power law strain hardening, a linear increase of flow stress with pressure and linear decrease with temperature. Also, note that the flow stress is zero for a temperature greater than the melting temperature. Also, the shear modulus  $\mu$  is nonlinear, Wilkins [15], and it depends on temperature, pressure, and material parameters as well as the relative volume  $V_r$ , and it is given as

$$\mu = \mu_0[1 - b_2\sigma V_r^{\frac{1}{3}} - b_3(\theta - \theta_0)] , \quad (213)$$

where  $\mu_0$  is the undamaged shear modulus  $\mu_0$  (i.e.  $\theta = \theta_0$  and  $\epsilon_u^p = 0$  then  $\mu = \mu_0$ ). The shear modulus  $\mu$  in Equation (213) is linearly increase with the pressure and linearly decrease with the temperature. Finally, the stress threshold for damage initiation is linearly proportional to the yield strength  $Y$  normalized by the lower bound of the yield strength  $Y_0$  through the material parameter  $\sigma_0^*$  which is given.

$$\sigma^* = \sigma_0^* \frac{Y}{Y_0} , \quad (214)$$

where  $\sigma_0^*$  is a material constant. That is the stress threshold for damage initiation (i.e. the stress limiting point before and after damage) is assumed to have similar behavior characteristics as the yield strength before and after damage (i.e.  $Y_0$  and  $Y$ ), and they are set to be proportional.

Kiselev and Yumashev [5] assumed that the dissipation damage  $D$  is

$$D = \int_0^t \frac{1}{\rho} (\tau_{ij} \dot{\epsilon}_{ij}^p + \Upsilon \dot{\gamma}^2 - \frac{q_i \theta_{,i}}{\theta}) dt , \quad (215)$$

where the time integral represent the accumulative process of damage. Note that, the dissipation damage parameter  $D$  is the dissipation function  $d$  defined in Equation (162) where the active stress  $t_{ij}$  is replaced by the deviatoric active stress  $\tau_{ij}$  defined in Equation (203). That is the dissipation damage  $D$  consist of the mechanical dissipation  $d_m$  representing the dissipation due to the plastic flow, the dissipation of continual failure  $d_f$  representing the dissipation due to the damage mechanism the continuum suffers, and the thermal dissipation  $d_\theta$  representing the heat energy dissipation which occurs from the hotter temperature to the colder temperature where

$$d_m \geq 0 , \quad d_f \geq 0 , \quad d_\theta \geq 0 . \quad (216)$$

That is, the mechanical dissipation  $d_m$ , the dissipation of continual failure  $d_f$ , and the thermal dissipation  $d_\theta$ , must always be positive or zero which mean that these dissipation quantities can be created but can not be destroyed, and they are irreversible similar to the entropy concepts. Note that, the dissipation damage  $D$  is an accumulative damage parameter in time, and it is represented in Equation (215) by the time integral.

Since an incremental approach is chosen to solve the governing equations with elastoplastic constitutive model numerically, the dissipation damage  $D$  computed also numerically. That is, the governing equations, which are the conservation of linear momentum Equation (150) and the heat transfer (i.e. energy balance) Equation (171), are solved using up-dated Lagrangian approach.

These governing equations are coupled thermal-mechanical system where the constitutive models are the linear Fourier's law defined in Equation (39) for the heat flux, thermoelasticity for the linear material response, and the Prandtl-Reuss elastoplastic flow rule for the elastoplastic material. Note that since the model is developed for a structure under impact, the yield criterion is function of pressure, temperature, and material constants. Thus, using the up-dated Lagrangian approach, the solution of the governing equations provide all the quantities needed to compute the dissipation damage  $D$  from Equation (215). Using the computed structural damage parameter  $\gamma$  to update the variables which are damage dependent, the next increment is carried on using the updated variables in a similar fashion and so on.

### 3 Conclusion

An overview of the thermodynamic definitions, concepts, and principles were presented. This overview of thermodynamics provided the necessary background needed to understand the model of failure. A summary of the essentials were presented as follow: concepts and definitions, balancing laws, thermodynamic equilibrium or thermostatic, and the thermodynamic process. These essentials are used to illustrate the development of the model of failure given by Kiselev and Yumashev [5], which is developed to analyze failure in a structural under impact loading.

For this thermodynamic model of failure, the substate variables used to characterize the failure model are the elastic strain  $\epsilon_{ij}^e$ , plastic strain  $\epsilon_{ij}^p$ , and an internal variable  $\gamma$  associated with the

damage dissipation in the continuum. Kiselev and Yumashev [5] assumes in their model of failure that the strain tensor can be written in two parts the elastic strain  $\epsilon_{ij}^e$  and the plastic strain  $\epsilon_{ij}^p$ . The elastic strain  $\epsilon_{ij}^e$  is a linear elastic strain, i.e. infinitesimal strain where the strain used is Cauchy strain tensor  $\epsilon_{ij}^e$ , and the corresponding stress is the Cauchy stress tensor  $\sigma_{ij}$ . Also, an incremental approach is used to solve the problem. Thus, an infinitesimal response for the stress-strain due to infinitesimal strain-displacement relations can be used even though the structure undergoing large displacement. That is the stress and strain tensors, for both the Eulerian and Lagrangian formulation, reduce to the Cauchy stress tensor  $\sigma_{ij}$  and the Cauchy strain tensor  $\epsilon_{ij}$ , respectively, which are referred to as the incremental Cauchy stress and strain tensors ( $d\sigma_{ij}$  and  $d\epsilon_{ij}$ ). Furthermore, the formulation of the model's governing equations use the Lagrangian representation where the up-dated Lagrangian is chosen to solve the problem numerically. The conservation laws and the first and second law of thermodynamics are formulated. The dissipation function  $d$  is defined using the second law of thermodynamic which consist of three terms. These three terms are the mechanical dissipation  $d_m$ , the dissipation of continual failure  $d_f$ , and the thermal dissipation  $d_\theta$ . This model imposed more restriction than the Clausius-Duhem inequality by forcing the mechanical dissipation, the dissipation of continual failure, and the thermal dissipation to be greater or equal zero. That is, dissipation quantities can be created but can not be destroyed. The free energy and free enthalpy is formulated based on thermoelasticity as the thermostatic state used to model the non-equilibrium thermodynamic process (i.e. non-equilibrium thermodynamic process is transiting from one thermostatic state to another). The constitutive model used is the Prandtl-Reuss which models elastoplastic isotropic homogenous material. The Jaumann stress rate is used in the formulation of the constitutive model since large deformation is considered, the plastic deformation is

not affected by the rigid body rotation and in the Jaumann stress rate model. Also, this model is formulated for elastoplastic isotropic homogenous material under impact loading where the yield becomes function of temperature, pressure, and material parameters. Hence, the yield criterion is based on the Steinberg-Gurson model which formulates the yield as a function of temperature, pressure, and material parameters. Finally, the dissipation damage parameter  $D$  which characterize the damage process is based on the dissipation function formulated in the second law of thermodynamic, i.e. similar to Clausius-Duhem principle. This dissipation damage parameter  $D$  is computed as a cumulative process in time in an incremental fashion. Finally, the solution of the governing equations including the constitutive models which are the linear Fourier's law for the heat flux, thermoelasticity for the linear material response, and the Prandtl-Reuss elastoplastic flow rule for the elastoplastic material obtain using up-dated Lagrangian approach.

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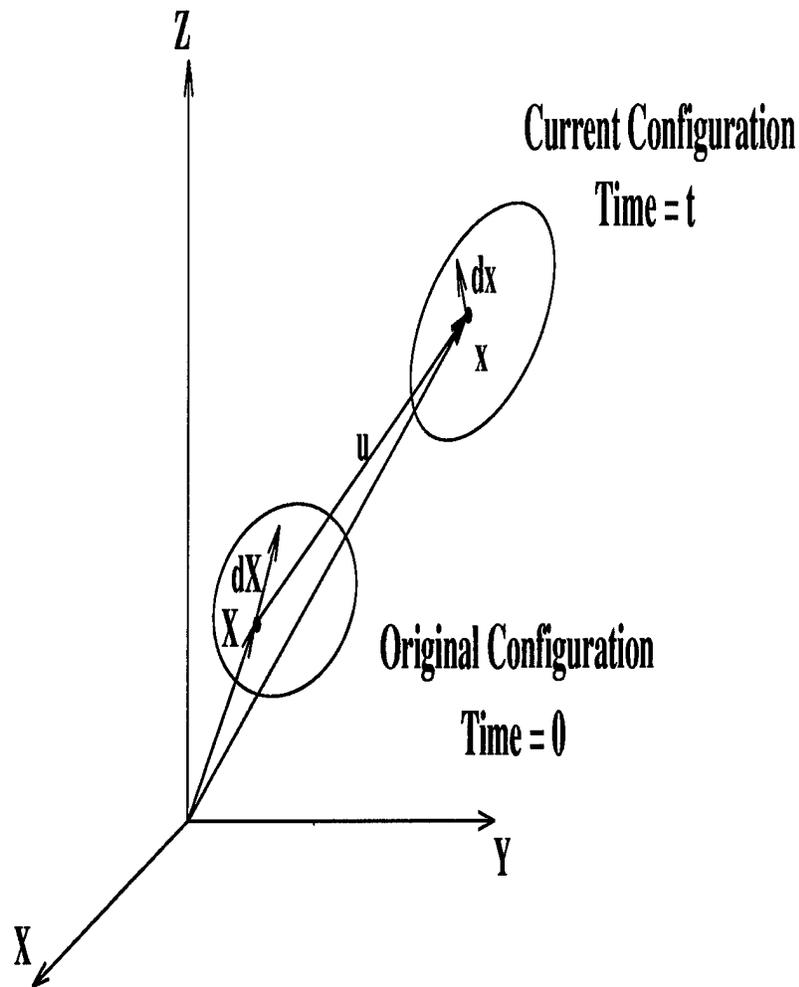


Figure 1:  $d\mathbf{X}$  is the deformation vector in the original configuration where  $\mathbf{X}$  is the position vector in Lagrangian description and  $d\mathbf{x}$  is the deformation vector in the current configuration where  $\mathbf{x}$  is the position vector in the Eulerian description.

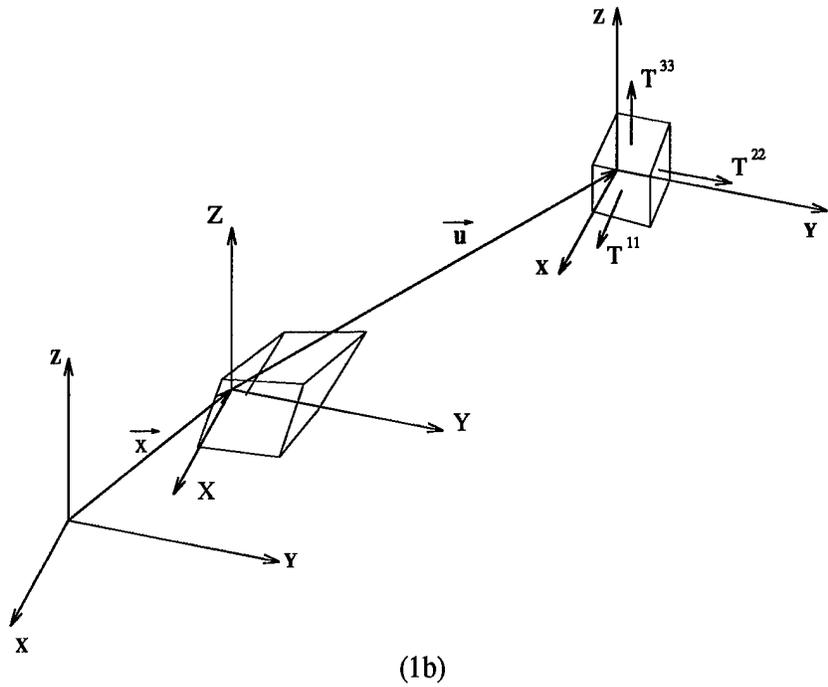
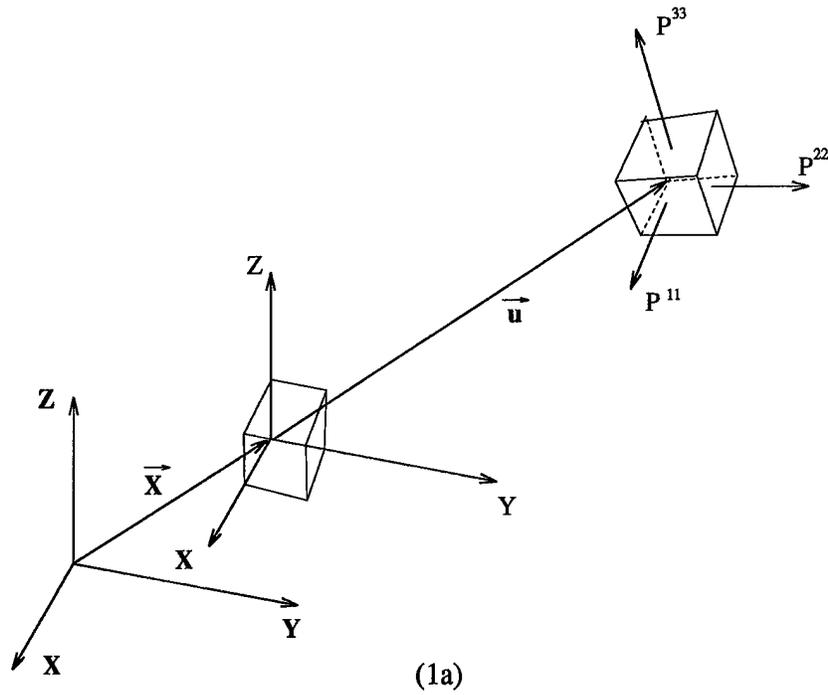


Figure 2: Stress tensor in Lagrangian and Eulerian systems: Figure 1a) second Piola-Kirchhoff stress tensor  $P_{IJ}$  and Figure 1b) Eulerian stress tensor  $T_{ij}$ .

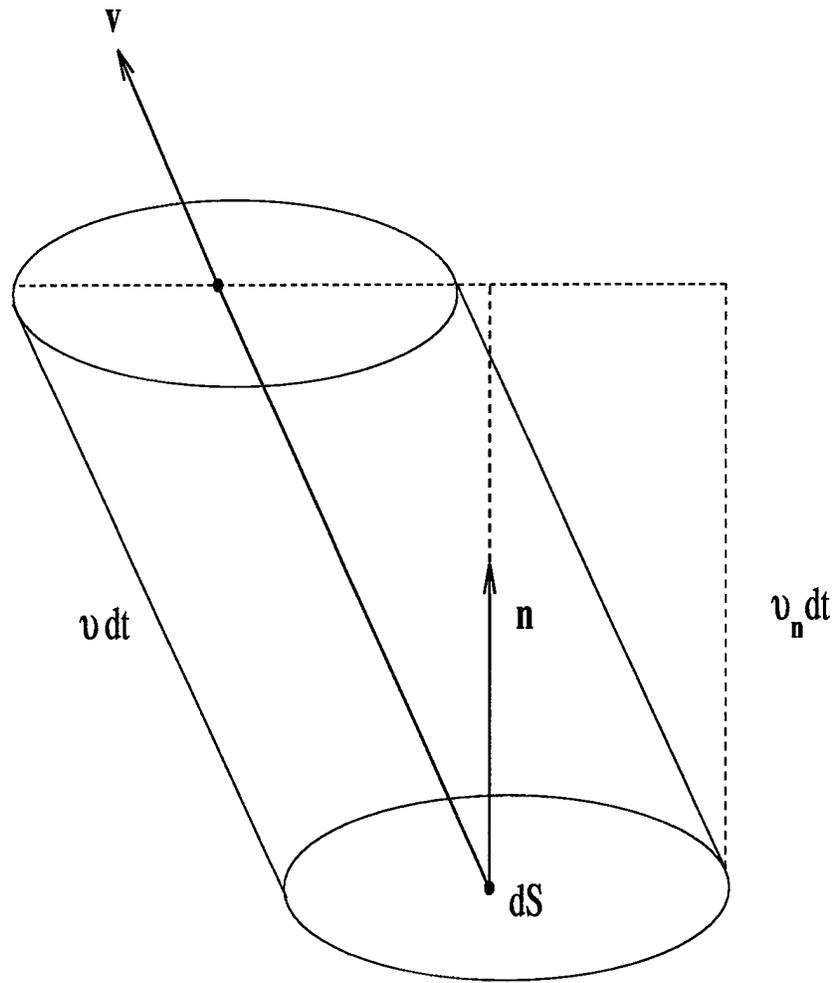
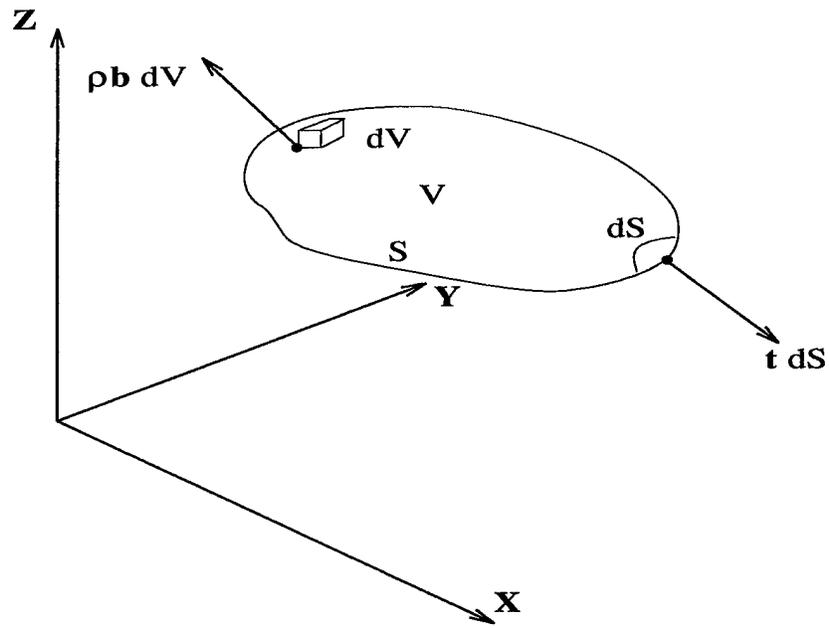
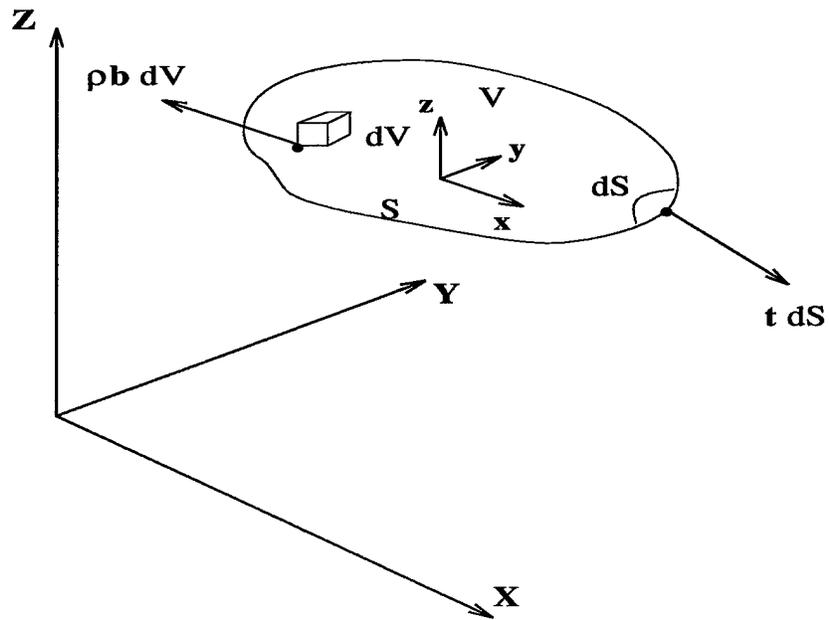


Figure 3: The flow of mass through element  $dS$  for a period of time  $dt$  where  $\mathbf{n}$  is the normal vector to the element  $dS$ ,  $\mathbf{v}$  and  $v_n$  is the velocity vector and the normal component of the velocity, and  $v dt$  is the distance the element  $dS$  travels.

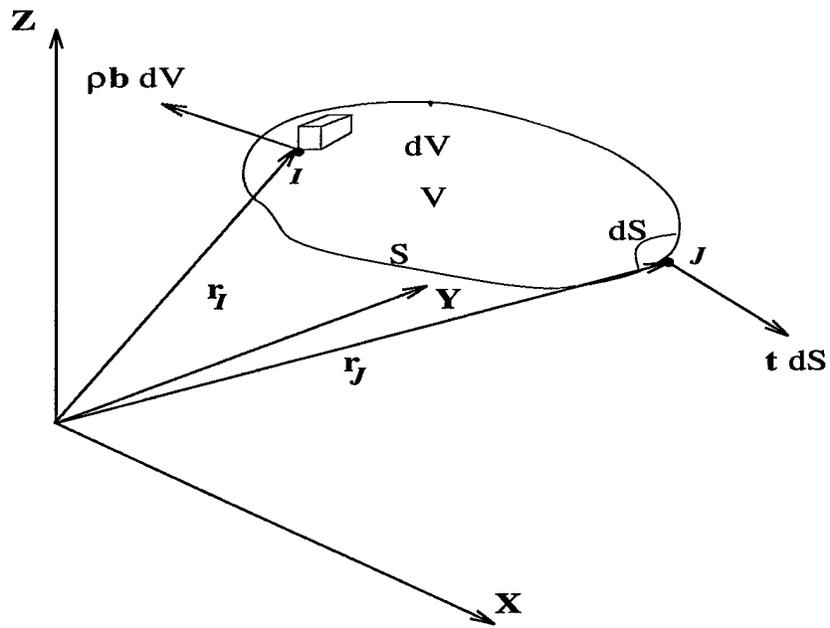


(4a)

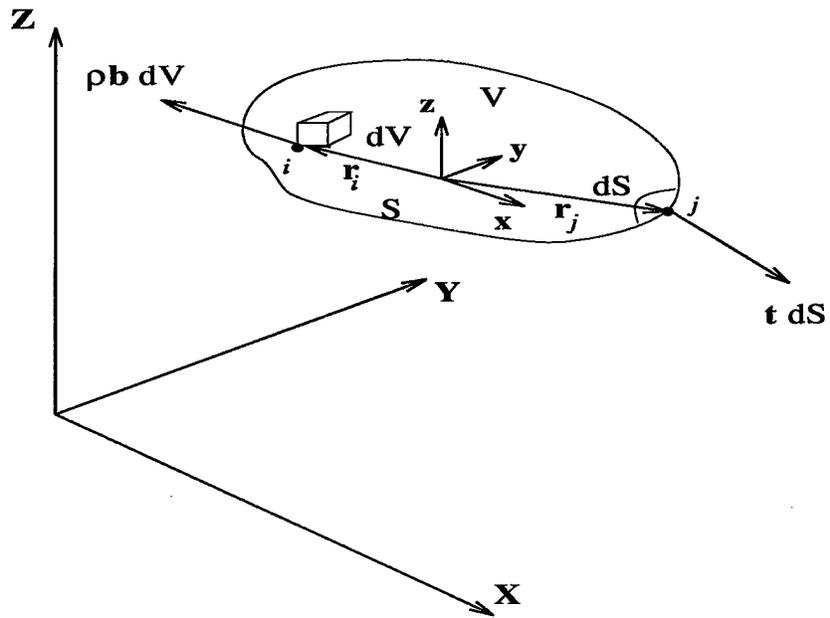


(4b)

Figure 4: The conservation of angular momentum: Figure 4a) is the conservation of angular momentum in the Lagrangian representation and Figure 4b) is the conservation of angular momentum in the Eulerian representation

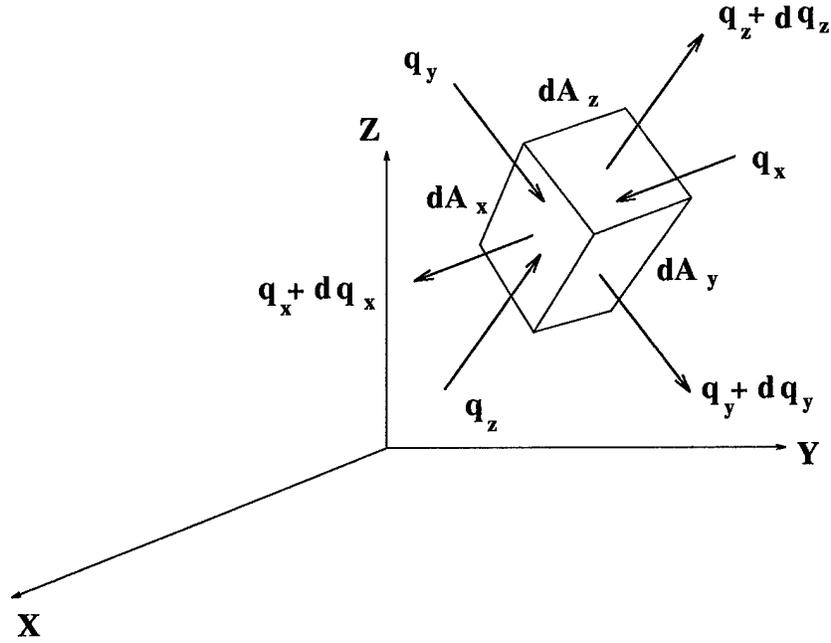


(5a)

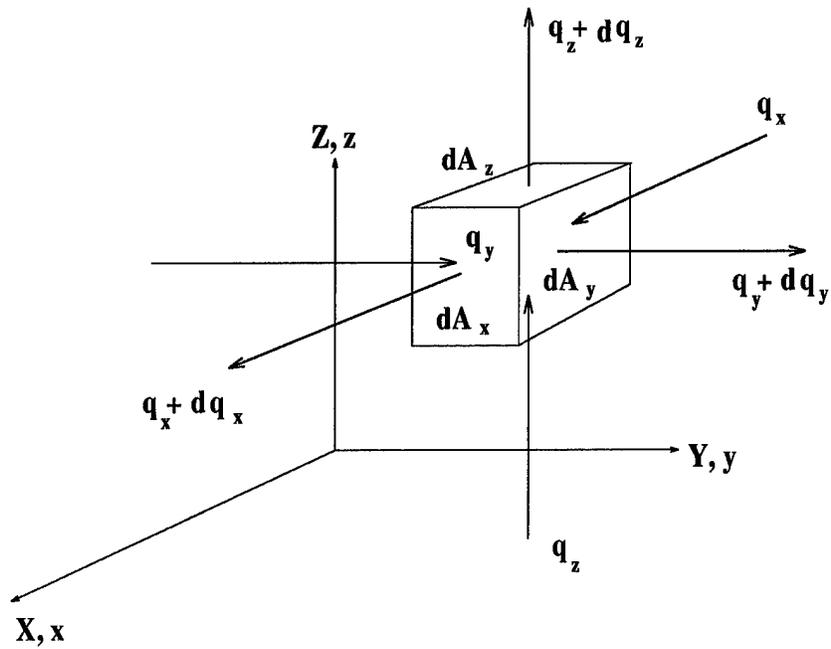


(5b)

Figure 5: The conservation of linear momentum: Figure 5a) is the conservation of linear momentum in the Lagrangian representation and Figure 5b) is the conservation of linear momentum in the Eulerian representation



(6b)



(6b)

Figure 6: The heat flow through the surface of the differential volume: Figure 6a) is the heat flow through the surface of the differential volume in the Lagrangian representation and Figure 4b) is the heat flow through the surface of the differential volume in the Eulerian representation

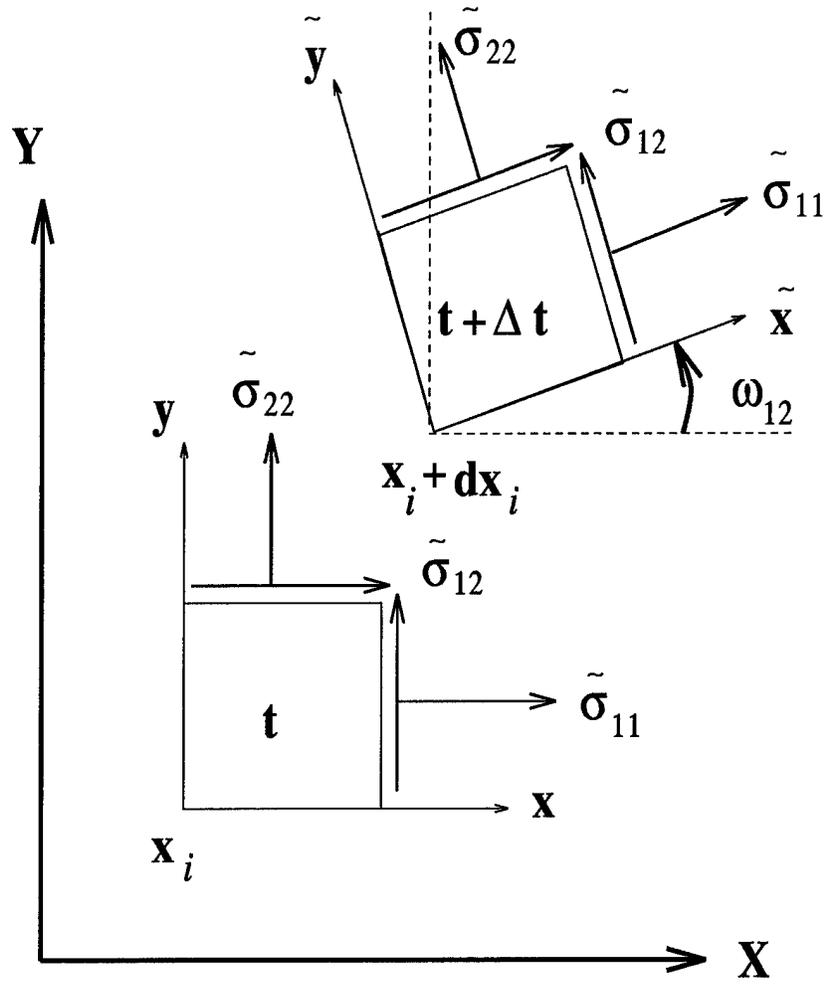


Figure 7: The stress components in the local coordinate system that translate and rotate with material point as it deformed during a time period from  $t$  to  $t + \Delta t$ .

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13. ABSTRACT (Maximum 200 words)  This report provides a prelude to the work developed by Smirnov et al considering the damage model of laminated composite materials. An overview of the thermodynamic definitions, concepts, and principles will be presented. This overview of the thermodynamics is necessary to provided the background needed to understand the damage model, which is based on thermodynamic principles. The essentials will be presented as follows: concepts and definitions, balancing laws, thermodynamic equilibrium or thermostatic, and the thermodynamic process. Furthermore, the essentials of the thermodynamics will be used to illustrate the development of the model of failure given by Kiselev and Yumashev. The Kiselev and Yumashev model will be discussed prior to Smirnov's damage model since both are similar in their postulation of damage for structures undergoing impacts, and are based on thermodynamic principles. However, they are different in that the former is developed for elastoplastic isotropic homogenous material, and the latter is developed for laminated composite materials based on viscoelastic constitutive laws. That is, the constitutive equations for an elastoplastic material will be discussed to illustrate the use of a thermodynamic model of failure first, then the constitutive relations that incorporate a time dependent viscoelastic laminated composite materials will eventually be added in a subsequent report.				
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