



# Historical review of internal state variable theory for inelasticity

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## ABSTRACT

A review of the development and the usages of internal state variable (ISV) theory are presented in this paper. The history of different developments leading up to the formulation of the watershed paper by Coleman and Gurtin is discussed. Following the Coleman and Gurtin thermodynamics, different researchers have employed the ISV theory for dislocations, creep, continuum damage mechanics (CDM), unified-creep-plasticity (UCP), polymers, composites, biomaterials, particulate materials, multiphase and multiphysics materials, materials processing, multiscale modeling, integrating materials science (structure–property relations) into applied mechanics formulations, and design optimization under uncertainty for use in practical engineering applications.

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## 1. Historical setting

Internal state variable (ISV) theory has been growing in its influence over the past 20–30 years. The confluence of increased computing power, finite element method developments, and experimental validation methods have positioned ISV theory to have great impact in the design of thermomechanical structural components and failure analysis. Fig. 1 shows a summary roadmap of the birth of ISV theory and how different phenomena and mechanisms have been brought into the ISV theory over the years.

What is ISV theory? Essentially, it is a material model (or constitutive model) that can capture the mechanical history of a material and be used to predict mechanical properties such as strength and failure of a material. It can be used for elastic behavior but its strength is for inelasticity, such as plasticity, viscoelasticity, viscoplasticity, creep, and damage. It really can be used for any material (polymer-based, ceramic-based, and metal alloys). The convergence of thermodynamics, kinematics, kinetics, and mechanics provided the impetus for the mathematical formality of ISV theory as presented by Coleman and Gurtin (1967). From that time, ISV theory was used to address different material systems over time.

## 2. Thermodynamics

The inelastic internal state variable (ISV) theory owes much of its development to the early thermodynamic works of Carnot (1824), Joule (1843), and Clausius (1850), which later lead to the development of state variable thermodynamics constructed by Helmholtz (1847), Maxwell (1875), Kelvin Thomson (1851), and Gibbs (1873a,b) in the late 19th century and early 20th century. The notion of ISV was morphed into thermodynamics by Onsager (1931) and was applied to continuum mechanics by Eckart (1940, 1948).

The basic idea behind the theory of an ISV is that, in order to uniquely define the Helmholtz free energy of a system undergoing an irreversible process, one has to expand the dimensions of the state space of deformation and temperature

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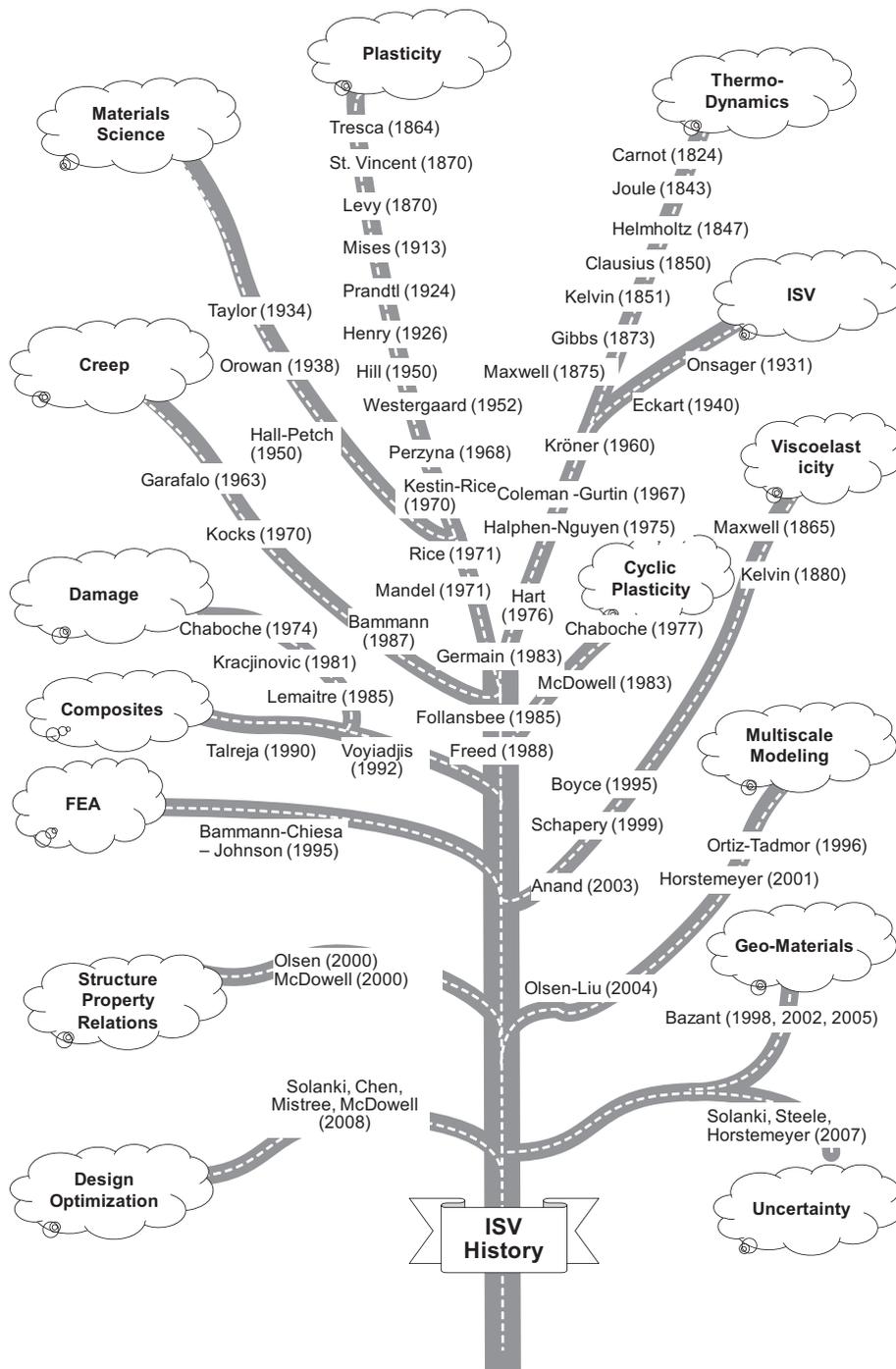


Fig. 1. Historical summary of different roads that formulated the modern internal state variable theory.

(observable state variables, “OSVs”, commonly employed in classical thermodynamics to study elastic materials) by introducing a sufficient number of additional state variables, ISVs, which are considered essential for the description of the internal structure of the material in question. The number of these variables is related to material structure and to the degree of accuracy with which one wishes to represent the material response. One can also use a Gibbs free energy to systematically quantify the internal state variables. In fact, special relations of the ISVs and OSVs can be realized by examining the converse relationship of the Helmholtz free energy and Gibbs free energy. Typically, the Helmholtz free energy is employed for solid materials and the Gibbs free energy for fluids.

The inelastic ISV formulation is a means to capture the *effects* of a representative volume element and not all of the complex *causes* at the local level; hence, an ISV will macroscopically average in some fashion the details of the microscopic arrangement. In essence, the complete microstructure arrangement is unnecessary as long as the macroscale ISV representation is complete (Kröner, 1960). As a result, the ISV must be based on physically observed behavior and constrained by the laws of thermodynamics. Coleman and Gurtin (1967) formalized the ISV theory with continuum theory and thermodynamics to provide the watershed paper for most of the viable theories that relate to different phenomena.

The thermodynamically-based constitutive equations that are used to capture history effects are cast in two classes. In the first class using hereditary integrals, the present state of the material is described by the present values and past history of observable variables (Lubliner, 1990). The second class is based on the concept that the present state of the material depends only on the present values of observable variables and a set of ISVs (Coleman and Gurtin, 1967). The second approach is more appropriate to solve a wide range of boundary value problems, and it is this form that we discuss in this writing.

Before we proceed in discussing the thermodynamics of ISVs, we must first briefly define the tensor notation. An underline indicates a first rank tensor (vector) for a small letter and a second rank tensor for a capital letter, i.e.  $\underline{v}$  and  $\underline{F}$ , respectively. A global Cartesian coordinate system is assumed so no distinction is made between the contravariant and covariant components. A first, second, and fourth rank tensor in the Einstein indicial notation form are given by  $v_i$ ,  $F_{ij}$ , and  $A_{ijkl}$ , respectively. Tensors are also denoted in bold face type in the text.

In thermodynamics the internal energy  $u$ , entropy  $s$ , heat flux  $\mathbf{q}$ , and the Cauchy stress  $\sigma$  are all considered state functions that can be determined by the state variables. The formulas that relate the state functions to the state variables are called *state equations* or *constitutive equations*. From a purely mechanical consideration, the only constitutive equation is that for the Cauchy stress  $\sigma$  or Piola-Kirchhoff stress  $\underline{\Sigma}$ .

For thermoelasticity one can expect that the state variables would be the deformation gradient  $\underline{\mathbf{F}}$  and the temperature  $T$  since here  $u$ ,  $s$ ,  $\mathbf{q}$ ,  $\underline{\sigma}$  and are determined completely by their current values. Thus, for an ideal thermoelastic behavior:

$$\begin{aligned} u &= u(\underline{\mathbf{F}}, T) & s &= s(\underline{\mathbf{F}}, T), \\ \mathbf{q} &= \mathbf{q}(\underline{\mathbf{F}}, T) & \underline{\sigma} &= \underline{\sigma}(\underline{\mathbf{F}}, T). \end{aligned} \quad (1)$$

This situation becomes much more complex if deformation is inelastic. For example, the stress of a plastically deformed solid cannot be determined by the current values of  $\underline{\mathbf{F}}$  only. The history of deformation is also necessary. Simple state equations or constitutive equations, such as Eq. (1) cannot describe correctly the plastic deformation of solids. It is necessary to know for a plastically deformed solid what other variables are needed to uniquely describe the current state. It is difficult to enumerate all the relevant state variables from macroscopic considerations and some assumption have to be made to use certain macroscopic observable variables as the representatives of the microscopic phenomena. Knowing this, the mathematical forms of the constitutive equations should be determined after the state variables are chosen. This involves the experimental evaluation and mathematical formalization.

The internal state variable (ISV) formulation first laid out by Coleman and Gurtin (1967) and later enhanced by Rice (1971), Kestin and Rice (1970) to solve the problem of specifying state variables. In this approach the current state of an inelastically deformed solid is postulated to be determined by the current values of  $\underline{\mathbf{F}}$ ,  $T$ , and a set of internal (or hidden) variables. The history of deformation is indirectly included in the evolution of these internal variables. The material response will be different if the values of the internal variables are different even though  $\underline{\mathbf{F}}$  and  $T$  are the same. We state this mathematically as

$$\begin{aligned} u &= u(\underline{\mathbf{F}}, T, \alpha_i) & s &= s(\underline{\mathbf{F}}, T, \alpha_i), \\ \mathbf{q} &= \mathbf{q}(\underline{\mathbf{F}}, T, \alpha_i) & \underline{\sigma} &= \underline{\sigma}(\underline{\mathbf{F}}, T, \alpha_i), \end{aligned} \quad (2)$$

where  $\alpha_i$ ,  $i = 1, 2, \dots, n$  are a set of  $n$  internal variables including mechanical, or thermal, or even electrical internal state variables. These variables can be scalars, vectors, or tensors, although they are also denoted by scalar symbols here. The specific physical meaning for each internal variable and the actual number  $n$  need to be chosen and identified for different materials and different conditions. Different choices result in different models as will be discussed later.

To gain a better physical understanding of the internal variables, let us look at the correlation between the inelastic behaviors of materials with their microscopic contents. When materials deform, the internal microstructure (an internal state variable) evolves. A correlation between microstructure and inelastic response was demonstrated by Motteff (1980) for type 304 stainless steel at 650 °C. Fig. 2 shows five microstructures from five specimens at different values of strain during tensile tests. One can see that the microstructure evolves and changes during deformation. The number of dislocations (the dark lines) increases from almost dislocation free state to a microstructure with a three dimensional dislocation cell-like structure. Two typical measures among many that could be used to characterize changes in the microstructure during deformation are the dislocation density and average cell size. The values of these variables can be correlated to a state of stress or strain on the tensile response curve. Thus, there is a correlation between the material microstructure and the mechanical response. Our objective is to use this type of information to enhance our understanding of material response and to develop material models.

In the approach of Coleman and Gurtin (1967), Coleman and Noll (1959) the Helmholtz free energy  $\psi$  is introduced in terms of the internal energy  $e$ , the entropy  $s$ , and the temperature  $\theta$  through the Legendre transformation as

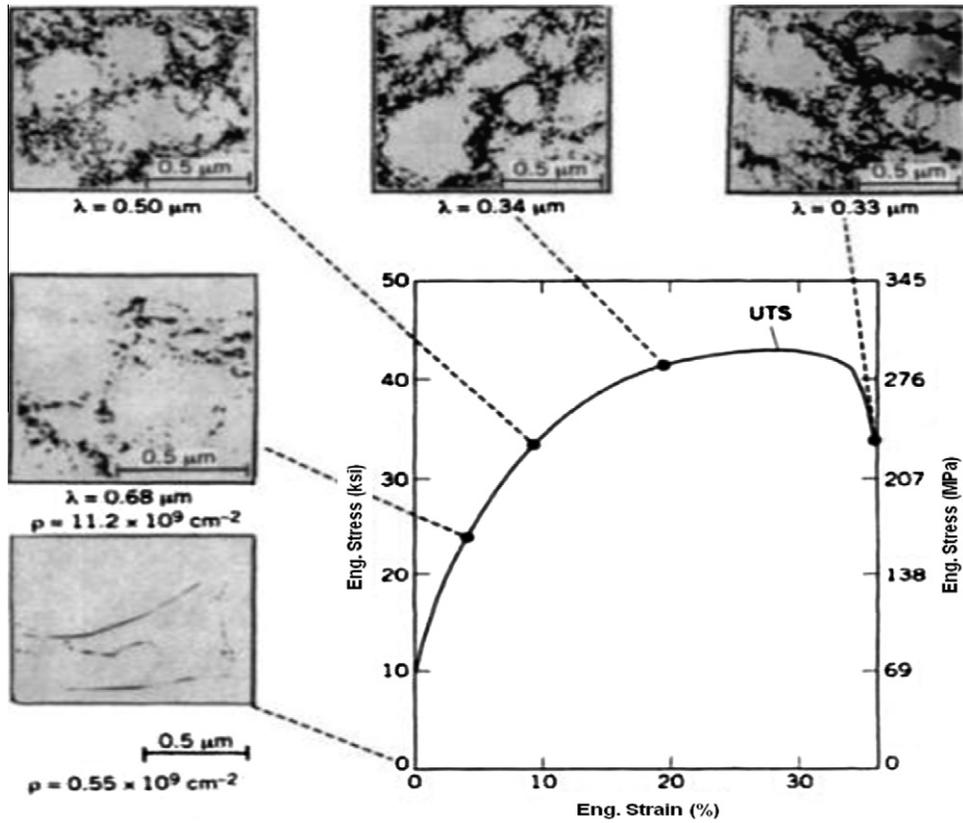


Fig. 2. Stress–strain behavior of type 304 stainless steel at 650 °C at a nominal strain rate of  $3.17 \times 10^{-4} \text{ s}^{-1}$ , together with the corresponding dislocation substructure at five different strain levels (Moteff, 1980).

$$\psi = u - s\theta. \tag{3}$$

Assumptions are now made concerning the dependence of the free energy on appropriate external and internal variables. For example, the simplest examples in plasticity are the elastic strain  $E_e$  and the temperature. To simplify the presentation of the concept, the small strain assumption is utilized such that the elastic strain is simply the total strain  $\underline{E}$  minus the “plastic” strain,  $E_p$ :

$$\underline{E}_e = \underline{E} - E_p. \tag{4}$$

We can thus assume:

$$\psi = \hat{\psi}(\underline{E}_e, \theta, \alpha_i), \tag{5}$$

where  $\alpha_i$  is a set of ISVs related to the quantities of interest such as defect densities such as dislocations or voids or diffusing species such as hydrogen. This assumption is then coupled with the reduced entropy inequality, to obtain thermodynamic restrictions on the form of the constitutive equations and the temporal rate equations for the state variables. The entropy inequality is generally assumed of a form:

$$\dot{\psi} + s\theta - \frac{1}{\rho} \cdot \underline{\sigma} \cdot \text{grad } \underline{v} + \frac{1}{\rho\theta} \cdot \text{grad } \theta \leq 0, \tag{6}$$

where  $\mathbf{q}$  is the heating,  $\sigma$  is the stress, and  $\text{grad } \underline{v}$  is the velocity gradient in which the symmetric part with the small strain assumption is simply equal to the total strain rate  $\dot{E}$ . Now since:

$$\dot{\psi} = \frac{\partial \psi(\underline{E}_e, \theta, \alpha_i)}{\partial \underline{E}_e} \cdot \dot{\underline{E}}_e + \frac{\partial \psi(\underline{E}_e, \theta, \alpha_i)}{\partial \theta} \cdot \dot{\theta} + \frac{\partial \psi(\underline{E}_e, \theta, \alpha_i)}{\partial \alpha_i} \cdot \dot{\alpha}_i \tag{7}$$

Substituting into the reduced entropy inequality, we get the following:

$$\left\{ -\frac{\partial \psi(\underline{E}_e, \theta, \alpha_i)}{\partial \underline{E}_e} + \frac{1}{\rho} \underline{\sigma} \right\} \cdot \dot{\underline{E}}_e + \left\{ \frac{\partial \psi(\underline{E}_e, \theta, \alpha_i)}{\partial \theta} + s \right\} \dot{\theta} + \frac{\partial \psi(\underline{E}_e, \theta, \alpha_i)}{\partial \alpha_i} \cdot \dot{\alpha}_i + \underline{\sigma} \cdot \dot{\underline{E}}_p - \frac{1}{\rho\theta} \mathbf{q} \cdot \text{grad } \theta \geq 0. \tag{8}$$

Therefore satisfaction of the reduced entropy inequality requires that the material is hyperelastic (stress is the derivative of the free energy with respect to the elastic strain); the entropy is negative in the derivative of free energy with respect to temperature; there is externally driven dissipation through the power associated with the stress and plastic strain as well as internal storage/dissipation through the power of internal stresses; and the entropy flux in this model is driven by the temperature gradient:

$$\begin{aligned} \underline{\sigma} &= \rho \frac{\partial \psi(\underline{E}_e, \theta, \alpha_i)}{\partial \underline{E}_e}; \quad s = - \frac{\partial \psi(\underline{E}_e, \theta, \alpha_i)}{\partial \theta}, \\ \frac{\partial \psi(\underline{E}_e, \theta, \alpha_i)}{\partial \alpha_i} \cdot \dot{\alpha}_i + \underline{\sigma} \cdot \dot{\underline{E}}_p - \frac{1}{\rho \theta} q \cdot \text{grad} \theta &\geq 0. \end{aligned} \quad (9)$$

To complete the system, constraint equations must be proposed to account for the extra degrees of freedom resulting from both the kinematics and ISVs. In particular, expressions are needed for the plastic strain rate  $\dot{\underline{E}}_p$  and the temporal evolution,  $\dot{\alpha}_i$ . In the case of a simple dislocation based model, these are given by expressions for the dislocation velocity and dislocation density evolution (e.g., storage minus recovery). The appropriate forms of these expressions as well as the associated parameters must be chosen to satisfy the above dissipation.

The question of equilibrium versus approximations with non-equilibrium states has been a fundamental question of research since the inception of ISV theory. One issue has been whether to use ISVs or extended OSVs to capture the appropriate physics. Lu and Hangoud (2007) for example proposed a hybrid model to capture internal damping by introducing ISVs and extended OSVs for nonequilibrium quantities within the thermodynamic fluxes. A recent Lagrangian formulation for non-equilibrium thermodynamics employing ISVs was that of Rahouadi et al. (2003), where the generalized Lagrangian coordinates correspond to the OSVs and ISVs of the time derivatives of the Gibbs potential.

### 3. Plasticity

As that history that led up to the Coleman and Gurtin (1967) work was proceeding, plasticity theory and the interconnections with materials science were evolving as well. The history of plasticity as a science probably began in 1864 when Tresca (1864) published his results on punching and extrusion experiments and formulated his famous yield criterion. Saint-Venant (1870), Levy (1870) building upon Tresca's work laid the foundation for the modern theory of plasticity. Over the next 75 years progress was slow and spotty, although important contributions were made by von Mises (1913, 1928), Hencky (1925), Prandtl (1924), and others. Only since approximately 1945 did a unified theory begin to emerge because of the fundamental continuum plasticity efforts of Prager (1945), Drucker (1949). Since that time, concentrated efforts by many researchers have produced a voluminous literature that has been growing at a rapid rate. In the 1950s excellent foundational works on plasticity were furnished by Hill (1948, 1950), Bishop and Hill (1951), Westergaard (1952), Kröner (1958). Drucker (1949) attempted a unified approach to plasticity based upon his definition of syability due to positive plastic work. This idea was further extended by Koiter (1960), Naghdi (1960) who proposed constitutive equations based upon Drucker's inequalities. Green and Naghdi (1965) formulated the classical theory of plasticity in the framework of modern continuum mechanics whereby the Second Law of Thermodynamics is invoked to determine restrictions on the form of the constitutive equations. Using this approach they were able to extend the classical theory to include large deformations and rate effects. The kinematic basis of Green and Naghdi's work was the assumption that the total strain could be decomposed into the sum of elastic and plastic strain tensors.

Lee and Liu (1967) and independently Mandel (1973) proposed an alternative approach by assuming the multiplicative decomposition of the deformation gradient into elastic and plastic parts resulting naturally into the velocity gradient decomposition into the sum of elastic and plastic parts. This decomposition has the identical structure of that proposed by Bilby (1954, 1955, 1956, 1958, 1960), but was utilized to describe very different phenomena. The multiplicative decomposition of the deformation gradient was later shown to result naturally into the additive decomposition of elastic and plastic strain as proposed by Green and Naghdi (c.f., Bammann and Johnson, 1987). The 1960s brought about much theoretical and experimental work (c.f., Phillips and Gray, 1961) to help lay the foundation for the future computational works that arose later. For example, Kondo (1952), Bilby et al. (1956, 1958), Kröner (1960) discussed Cartan's torsion tensor in the context of what would now be called "geometrically necessary dislocations". It was Kroner's work (1960, 1961, 1963) in which the notion of an internal variable representing dislocations was first qualitatively described. Mind you, the Coleman and Gurtin (1967) formalism had not been introduced yet with consistency of all of the governing equations. However, he stated that there we could include internal state variables to represent all of the important "effects" without having to address all of the "causes". It was Teodosiu (1969) who connected the intermediate configuration with the incompatibility of geometric necessary dislocations and scalar dislocation density as an ISV, and first utilized the Coleman-Gurtin thermodynamic framework to describe dislocation based inelasticity. With the advent of computers many plasticity models blossomed with time and temperature dependent formulations including the relation of internal state variable theory within the context of plasticity by Kestin and Rice (1970), Rice (1971), Mandel (1971).

In the 1970s, researchers in France laid the foundations for elastoviscoplasticity internal state variable theory starting with Mandel (1971). Halphen and Nguyen (1975) introduced the mathematical structure of finite deformation plasticity theory with ISVs that was based upon either a free energy potential and a dissipation potential. They used convex analysis and

introduced the important concept of generalized standard materials. A great summary of this work was summarized by Germain et al. (1983).

Also in the 1970s the details of the crystal plasticity discussions joined the worlds of materials and mechanics, c.f., Kocks (1970). In the 1970s (c.f., Krempl, 1975) and 1980s (c.f., Bammann, 1984) unified-creep-plasticity (UCP) theories were a main focus along with the development of various internal state variable theories on various aspects of plasticity. The notion that a dislocation did not know if it was in a state of constant uniaxial stress (creep) or constant uniaxial strain (plasticity) remotely led to these formulations. Prior to this, different creep formulations were presented, mainly from the materials science community focusing on the flow rule. Probably the first development of an ISV theory for creep was that of Murakami et al. (1981, 1983) followed by Henshall and Miller (1990), Bammann (1990), and others. Plasticity on the other hand had been focusing on the theoretical and numerical aspects of flow with a yield surface.

In the 1990s the application of using internal state variable theory in the unified-creep plasticity context required much research on numerical implementation and analysis. As the new century dawned, the inclusion of the structure–property relations into the internal state variable in solving complex boundary value problems for practical engineering problems.

We start by defining roughly and intuitively what is meant by a metal flowing plastically. If one takes a thin strip of a metal such as aluminum and clamps one end and applies a bending moment to the other end, the end of the strip will deflect. Upon removal of this force, if this force is not too large, the end of the strip will spring back to its original position, and there will be no apparent permanent deformation. If a sufficiently large load is applied to the end, the end will not spring back all the way upon the removal of the load but will remain permanently deformed, and we say that *plastic flow* has occurred.

#### 4. Materials science (mechanism quantification for structure–property relations)

Perhaps the materials science community has had the greatest impact on quantifying the physical mechanisms for ISV theory. When addressing the physical admissibility postulate for continuum theory, the materials science community has provided the physical understanding of the main deformation mechanisms. It is inherent within the materials science community to study the microstructural mechanisms and associated length scale effects, although they have not necessarily focused on ISV modeling. The terminology typically used in the materials science community is “structure–property” relations. Essentially, it is the different structures within the material (grains, particles, defects, inclusions, etc.) that dictate the performance properties of the materials (Olson, 1998; Olson, 2000).

Different scale features give different scale mechanical properties. At the smallest level, the lattice parameter is a key length scale parameter for atomistic simulations. Since atomic rearrangement is intimately related to various types of dislocations, Orowan (1934), Taylor (1934), Polyani (1934), Nabarro (1952) developed a relationship for dislocations that related stress to the inverse of a length scale parameter, the Burgers’ vector (1939), which laid the foundation for all plasticity theories. Nabarro (1952) also showed that the diffusion rate is inversely proportional to the grain size, another length scale parameter. Hall (1951), Petch (1953) related the work hardening rate to the grain size. Ashby (1971) found that the dislocation density increased with decreasing second phase particle size. Frank and Read (1949, 1951, 1953) showed a relation with a dislocation bowing as a function of spacing distance and size. And (Hughes et al. (1991, 1992) discovered that geometrically necessary boundary spacing decreased with increasing strain, although it continued to increase the work hardening rate.

Orowan (1934) considered the mean effect rather than individual aspects of dislocation motion in an attempt to describe macroscopic plastic flow. He postulated that the rate of plastic deformation  $\dot{\epsilon}_p$  was determined by the number of dislocations per unit volume and their average rate of propagation:

$$\dot{\epsilon}_p = \rho b \bar{v}, \quad (10)$$

where  $\rho$ ,  $\bar{v}$ , and  $b$  are the average mobile dislocation density, dislocation speed, and Burgers vector, respectively.

Johnston and Gilman (1959) experimentally measured the average dislocation velocity as a function of stress in lithium fluoride crystals and proposed an empirical relationship to describe their results. They also assumed the rate of increase of mobile dislocations is proportional to the flux of mobile dislocations and the rate of immobilization is proportional to the square of the mobile density. Integrating this equation, in conjunction with their expression for the dislocation speed and using Orowan’s relationships under the assumptions that all dislocations are mobile, the yield phenomenon in LiF crystals was accurately predicted.

This success led to the widespread adoption of what Argon (1968) calls the “dilute solution” approach to dislocation motion. In this approach dislocations are assumed to move in a quasi-viscous manner under the action of an applied stress. The velocity of the motion is determined by the lattice resistance or friction. Interactions between dislocations are assumed negligible or accounted for by an effective stress (applied stress minus back stress). Hardening, instead of being related to a rate mechanism, is defined in terms of the effective stress.

Along these lines, Webster (1966a,b) assumed that the time rate of change of dislocation density was due to multiplication and immobilization processes in a manner analogous to Gilman. Substituting an empirical relationship for the dislocation velocity in which he assumed the speed depended exponentially on the applied stress, resulted in Eq. (11a) as the following:

$$\dot{\rho} = n + \alpha\rho - \beta\rho^2, \quad (11a)$$

$$\frac{d\rho}{d\varepsilon_p} = c_1 \frac{1}{\lambda} - c_2\rho = c_1\sqrt{\bar{\rho}} - c_2\rho, \quad (11b)$$

where  $n$ ,  $\alpha$ , and  $\beta$  are independent of dislocation velocity and functions of only stress and temperature. Integrating this expression under constant stress and temperature conditions and assuming all dislocations are mobile, Webster predicted Stage I and II creep in single brass and aluminum oxide crystals. For a complete review of this approach see Gilman (1966, 1968, 1969). Later, Mecking and Kocks (1981) modified Eq. (11a) to better capture the hardening-recovery as in Eq. (11b), where  $C_1$  and  $C_2$  are hardening and dynamic recovery coefficients, respectively. About the same time, Bammann and Aifantis (1982) proposed that an ISV for dislocations is required to complete the mass and momentum balance laws as opposed to simple temporal evolution equations.

The formalism for nonlinear relationships using internal variable theory was realized in Coleman and Gurtin (1967). Although internal variables in thermodynamics were previously used by Onsager (1931a,b), Valanis (1966), for example, the theory was formalized within the realm of modern nonlinear continuum mechanics in the work of Coleman and Gurtin. Lubliner (1972, 1973, 1974) showed that a material, whose thermodynamic state is described by internal variables obeying evolutionary equations, possesses the property of fading memory under certain conditions (if the evolutionary equations are differentiable and if the matrix of their partial derivatives with respect to the internal variables is negative definite. These, in fact, are fairly broad conditions).

In the internal variable approach, the mechanical state at a material point in a body is described in terms of hidden or internal variables in addition to the usual observable external variables such as temperature and deformation. Even though extensive work has been conducted in this area, there is not universal agreement on the number and kind of internal variables to be used. McDowell (2005) argued that of the different continuum postulates for constitutive relations, particularly with respect to internal variables, should have physical admissibility based upon experimental observation as the first priority.

Shortly after Coleman and Gurtin's work (1967), Perzyna and Wojno (1968) formulated a rate dependent plasticity theory by assuming the components of an inelastic deformation as an internal variable. No specific evolutionary equations were postulated and no examples solved. Along similar lines Bhandari and Oden (1973) presented a rate dependent theory in which they assumed an inelastic strain tensor (similar to that of Perzyna and Wajno) and a set of second order dislocation density tensors motivated by Kröner (1962, 1965)) constitute the internal variables. In their formulation, no specific form was given for the evolutionary equations.

Kratochvil and Dillon (1969) formulated in internal variable theory in which the internal variables comprised a finite number of second order dislocation arrangement tensors. This was a rate independent theory in that no thermally activated or other viscous type motion was assumed. They assumed an elastic–perfectly plastic material response by requiring the slope of the dislocation speed versus sheer strain curve to approach infinity. In solving a specific example, an explicit model was assumed. The second order dislocation arrangement tensors were reduced to two scalar parameters representing the dislocation density, dislocation entanglements, and an associated yield function. This work was extended by Kratochvil and DeAngelis (1971) to include rate dependant processes by assuming thermally activated motion dependent upon the local shear stress (applied shear stress minus back stress due to dislocation pileup in a glide plane). The model was then applied to the torsion of a titanium shaft. Kratochvil (1973) further extended this model to include finite strain by adopting the deformation gradient proposed by Lee and Liu (1967). Following Gillis and Gilman (1965) an exponential dependence of the dislocation speed on shear stress was assumed and the model was applied to the solution of a single crystal with only one slip system operative.

Approximately at the same time, Rice (1970, 1971) assumed that the plastic behavior of metal arises as a consequence relative to internal flip displacements of the crystallographic plane due to dislocation motion. By assuming that the rate of slip was time-dependent and that the resolved shear stress acting on the flip system was the thermodynamic driving force of the dislocation, the plastic strain components were derived from a potential function of stress. Along these lines, Zarka (1972) derived specific forms for plastic and viscoplastic potential for monocrystals and polycrystals. In a series of papers Teodosiu et al. (1976a,b) assumed that scalar tensorial variables could represent the total dislocation density and the concentration of point defect as their internal variables. This model incorporated many of the physical concepts of dislocation motion at the time. Although recovery was neglected, it was a rate dependent theory. The plastic strain rate was related to dislocation motion by Orowan relation (1934) and an orientation tensor similar to the Schmid (1926) orientation tensor. A local yield condition in terms of the resolved shear stress on a glide plane was specified, although only a general form for the backstress was assumed. This condition was imposed upon both the constitutive equations for the dislocations speed as well as the evolutionary equation for the dislocation density. For the evolutionary equation of the point defects, diffusion was neglected and only thermally activated motion was assumed. The evolutionary equations for both internal variables were related to derivative of Rice (1970) thermodynamics potential with respect to the thermodynamic forces. Although specific equations for the internal variables were not considered, an explicit expression for the dislocation speed was proposed based upon time that a dislocation corresponded to the velocity between obstacles. One key point from the thermodynamics was that the evolutionary equation for the dislocation density depended only upon the elastic strain through the resolved shear stress.

Another model considering the dislocation density as an internal variable was presented by Hahn and Jaunzemis (1973). Hahn and Jaunzemis derived a 3-D relationship similar to Orowan's equation (1934), relating the plastic strain rate to the dislocation density. By considering a local stress determined by the applied resolved shear stress minus a backstress, a generalized form of Prager's (1945) kinematic hardening law was established. Based on the specific evolutionary equations for the immobile and mobile scalar dislocation densities from Gilman (1969), the simple extension of a rigid-viscoplastic body under isothermal conditions with an operative slip system was solved for finite deformations based upon an inverse procedure.

Kelly and Gillis (1974a,b) assumed the Gibbs thermodynamic potential was a function of the dislocation density and following Coleman and Gurtin postulated an evolutionary equation for this quantity. They also assumed Orowan's relation for the plastic strain rate which was extended to three dimensions by using the Schmid orientation tensor:

$$\dot{\epsilon}_p = \sum \rho^{*(i)} v^{*(i)} b^{(i)} \mu^{(i)}, \quad (12)$$

where  $\rho^*$ ,  $v^*$  are the mean mobile dislocation density and speed, respectively,  $b$  is the Burgers vector and  $\mu$  is the Schmid orientation tensor:

$$\mu^{(i)} = \frac{\mathbf{n}^{(i)} \otimes \mathbf{b}^{(i)} + \mathbf{b}^{(i)} \otimes \mathbf{n}^{(i)}}{2}, \quad (13)$$

which reduces to Schmid's law (1926) for a single slip system in a single crystal under uniaxial tension. This is a symmetric tensor motivated by the dislocation density tensor to describe the dislocation state and hence the tensorial characteristics of the plastic strain rate at a point in the body. Kelly and Gillis (1974a,b) assumed an evolutionary equation for the speed based upon the empirical work of Gilman (1968, 1969) and his followers. Example problems in one dimension were solved including cyclic loading at constant strain rate. The method compared well with experiment and even predicted the Bauschinger (1886) effect in the cyclic loading case.

## 5. Unified creep-plasticity (UCP)

Starting in the 1970s (c.f., Bodner and Partom, 1975) with a major emphasis in the 1980s a major focus was on combining the materials science flow rules for creep with flow rules from plasticity. This effort forced different modeling frameworks together in a hodge-podge manner; however, ISV theory could join both ideas fairly rigorously. As a result, ISV theory started to gain influence as researchers employed the framework for unified-creep-plasticity (UCP) theories. Inherent within the notion was UCP ISV theory Marchand and Moosbrugger (1991) reviewed the models that included isotropic and kinematic hardening laws and discussed the applicability to proportional and nonproportional loadings and ageing. Most of the modern models in the UCP context were birthed from the creep work of Garofalo (1963) for the flow rule or the anisotropic creep model of Malinan and Khadjinsky (1972). Creep rules were introduced as ISVs but independent of plasticity at first. For example, Astafev (1987), McCartney (1981) introduced ISV theories for primary and secondary creep related to metals that addressed multiaxial and time-dependent stress and strain states. The well-known concepts of elastic, anelastic and plastic strains followed naturally from the theory. Cocks and Ponter (1991) developed an ISV theory with the thermodynamic structure focused on creep and higher rates of deformation of single crystal aluminum focusing on an expansion of dislocation loops through a network of sessile dislocations. Later, Allen and Beek (1985) reviewed different ISV models for metals and demonstrated the usage for nickel-based superalloys, which experience fairly high temperatures in their application space. For solder, Rist et al. (2006) pursued an ISV theory that focused on creep. In this work, they demonstrated that the high temperature, long term behavior of dislocations (related to creep) for monolithic tin and multiphase materials.

One of the early UCP ISV models was that of Hart (1976, 1984), who introduced an internal state variable model to capture dislocation glide and their interactions to rationalize the phenomenological features of inelastic deformation for steel alloys. Here, the relation among the applied stress, the internal stress, and the glide friction stress was derived as the internal stress was shown to be linearly proportional to a stored anelastic strain. Recently, Garmestani et al. (2001) employed the Hart model in examining transient behavior in cyclic loadings, and Kim et al. (2004) employed the Hart model to capture the temperature dependence of the plastic deformation of a titanium alloy.

The mechanical threshold stress (MTS) ISV model was based upon the work of Kocks (1970) in which different stresses arose from different internal structures but were basically an isotropic hardening formulation. Follansbee et al. (1985, 1986, 1988, 1990) first applied the MTS model to nickel-carbon based alloys showing the effects of history on hardening and dynamic strain ageing, then they applied it to many materials. Since then, this ISV modeling framework has been routinely used at Los Alamos National Laboratory for metal alloys.

The Chaboche (1977, 1983), Chaboche and Rousselier (1983), Lemaitre and Chaboche (1985), Chaboche (1989) ISV model included isotropic and kinematic hardening variables to capture the Bauschinger (1886) effect and cyclic hardening. Chaboche et al. (1991) discussed the thermodynamic foundation for ISVs for three fundamental ISVs (a tensorial backstress arising from kinematic hardening and scalar drag and yield strengths for isotropic effects). All three evolved according to competitive processes between work hardening, deformation induced dynamic recovery, and thermally induced static recovery. The evolution of internal state can also include terms that vary linearly with the external variable rates. Chaboche (1993) later discussed for each hardening process, the separation of the total plastic work into energy dissipated as heat and

energy stored in the material. Fuschi and Polizzotto (1998) illustrated the existence of a saturation surface in the internal variables space as a consequence of the energy boundedness for an associative flow rule that can be stored in the material's internal microstructure. For the nonassociative case, under a special choice of the plastic and saturation potentials and through a suitable parameter identification, the well-known Chaboche model was reproduced.

The early UCP models were phenomenologically dislocation-based and encompassed many of the aspects of previous models, but were not specifically formulated in the thermodynamic format of Coleman and Gurtin (1967). These models were developed to predict deformation that encompassed both plasticity and creep, were dislocation based, predicted many of the aspects of plasticity without the introduction of a yield surface and avoided the creep models that were popular at the time that included "time" as a specific variable in the formulation. A summary of some of the models prevalent at that time is given in a report given by Jones et al. (1982) wherein they describe a skeletal structure that was common to all of these models. It is a structure that is still common among many of the thermodynamic based internal state variable models. The models were all small strain formulations in that it was assumed that the elastic strain rate or velocity gradient could be decomposed into the sum of elastic and plastic parts:

$$\underline{d} = \underline{d}_e + \underline{d}_p, \quad (14)$$

where  $\underline{d}$ ,  $\underline{d}_e$ ,  $\underline{d}_p$  are the total, elastic and plastic stretching tensors (symmetric part of the velocity gradients) or strain rates, respectively. Although Bilby (1956), Kröner (1960), Lee and Liu (1967) introduced the multiplicative decomposition of the deformation gradient earlier in which the associated elastic and plastic velocity gradients could be defined similar to Eq. (14), it was not generally employed in practice. At that time, the models assumed an elastic stretching tensor and the Cauchy stress:

$$\dot{\underline{\sigma}} - \underline{w}\underline{\sigma} + \underline{\sigma}\underline{w} = \lambda \text{Tr} \underline{d}_e + 2\mu \underline{d}_e, \quad (15)$$

where the Jaumann rate of stress was employed in terms of the total spin (skew part of the velocity gradient)  $\underline{w}$ . Eq. (15) was first formulated as a hypo-elastic constitutive relation but follows naturally when hyperelasticity is formulated with respect to the natural (intermediate) configuration, linearized and pushed forward to the current configuration. The flow rule is generally motivated by an equation for the dislocation velocity and hence is usually a power law, hyperbolic sine, or exponential function of the magnitude of the deviatoric stress and the state variables such as

$$\underline{d}_p = f \begin{cases} \text{Sinh} \left[ \frac{|\underline{\sigma}' - \underline{\alpha}| - \kappa}{V} \right], \\ \text{Sinh} \left[ \frac{|\underline{\sigma}' - \underline{\alpha}|}{V\kappa} \right], \end{cases} \quad (16)$$

where  $f$  and  $V$  were temperature dependent parameters and  $\alpha$  is a tensor variable emulating the kinematic hardening variable of classical plasticity enabling the prediction of softening upon unloading or other load path direction change. The scalar variable  $\kappa$  is an internal state variable representing "drag stress" or internal strength and appeared either in the denominator of the flow rule or the numerator in models such as overstress models such as the model of Krempl (1975). Evolution equations were prescribed for the ISVs, motivated by dislocation evolution and therefore generally were cast in a hardening minus recovery format:

$$\dot{\underline{\alpha}} - \underline{w}\underline{\alpha} - \underline{\alpha}\underline{w} = h\underline{d}_p - r(\underline{\alpha})\underline{\alpha}, \quad (17)$$

$$\dot{\kappa} = [H - R(\kappa)]|\underline{d}_p|, \quad (18)$$

The first usage of these types of ISV models for finite element codes in the solution of large scale structural problems was at Sandia National Labs in Livermore, CA in the early 1980s. The problems of implementing these types of models incurred mathematically stiff differential equations associated with the expression for the flow rule  $\underline{d}_p$ . This stiffness, while physically observed in measurements of the dislocation velocity by Gilman et al. (1969) and necessary to capture the observed mechanical "yield stress" without the specification of the hypersurface in stress space (yield surface) of classical plasticity, is still a source of problems in the mathematical implementation of these ISV models today and results in reduced time or strain increments in finite element calculations.

The basis for the Sandia National Laboratories ISV finite element simulations was based upon the plasticity model of Bammann (1984, 1987, 1990). The Bammann ISV model (1984, 1987, 1990) started with dislocation density evolution equations that captured the work hardening of a metal alloy. The key point in the Bammann formulation was having two dislocation density evolution ISVs: one for statistically stored dislocations introducing isotropic hardening and one for geometrically necessary dislocations for kinematic hardening. Later, the Cocks and Ashby (1980) creep rate was introduced into the ISV formalism (Bammann and Aifantis, 1989) to capture the damage evolution as the void volume fraction in the context of UCP. In Bammann et al. (1993) the ISV model integration into finite element codes and engineering examples of analysis and design are given to demonstrate the capability. It has been used to quantify reverse loads for different metals (Bammann and Dawson, 1993), complex boundary value problems, (Horstemeyer and Revelli, 1996), forming problems (Horstemeyer, 2000), and high rate phenomena (Bammann et al., 1990), thermomechanical materials processing (Guo et al., 2005), metal cutting (Guo et al., 2006), and micromachining (Guo et al., 2008).

In the context of UCP ISV theories, the postulate of a local continuum point has been argued to be at odds with the physical nature of dislocations inducing inelastic behavior in metals. Even before considering dislocations in metals for nonlocal or gradient theories, the [Cosserat brothers \(1913\)](#) introduced the notion of stress and strain gradients in a continuum formulation. Although [Cosserat and Cosserat \(1909\)](#) introduced the notion of stress gradients for added degrees of freedom in a continuum formalism, it was really [Eringen \(1967, 1968\)](#) who laid the foundation for nonlocal and gradient plasticity theories. However, the notion of using these methods since they typically try to model effects of dislocations that are imbedded within the work hardening ISVs not the OSVs. [Bammann and Aifantis \(1981\)](#) first introduced a dislocation gradient for capture work hardening. Recent examples include such works of [Polizzotto and Borino \(1998\)](#), [Cimmelli and Rogolino \(2001\)](#), [Dorgan and Voyiadjis \(2003\)](#), [Santaoja \(2004\)](#), [Marotti De Sciarra \(2004; 2008; 2009\)](#), [Maugin \(2006\)](#), [Abu Al-rub et al. \(2007\)](#), [Ricci and Brünig \(2007\)](#), [Abu Al-rub \(2008\)](#), [Forest \(2009\)](#). We note that the context here is the use of gradients and nonlocal theories with ISVs, not OSVs. Hence, we do not include the strain gradient work of [Dillon and Kratochvil \(1970\)](#), [Fleck et al. \(1994\)](#), and many others since strain is an OSV.

## 6. Materials processing (history effects)

Because the materials science community focused on the development of materials and tied the process-to-structure-to-properties, the inherent history effects of the materials processing was an opportunity for the use of ISV theory (see [Olson, 1998, 2000](#); [Horstemeyer and Wang, 2003](#)). The use of ISV theory was only possible in the context of finite element analysis as the boundary value problem needed to be resolved. Probably the first effort to apply a plasticity ISV model was that from [Eggert and Dawson \(1987\)](#), who employed the ISV Hart model to model the rolling process. Later, [Brown et al. \(1989\)](#) used a different ISV model with one isotropic ISV hardening equation to capture hot rolling deformation. Based on the [Eggert and Dawson \(1987\)](#) work. [Maniatty et al. \(1991\)](#) employed a polycrystalline plasticity model with ISV hardening equation to model rolling and extrusion. Using a higher length scale model, Later, [Wang \(1995\)](#) studied the evolution of matrix strength and porosity during hot rolling of aluminum metals by using a multiple ISV constitutive theory within finite element analysis. Also for hot rolling of aluminum, [Sellars and Zhu \(2000, 2003\)](#) used rate equations for ISVs to account for dislocation density, subgrain size, misorientation between subgrains, and subsequent recrystallization behavior for dynamic deformation conditions. [Karhausen and Roters \(2002\)](#) used an ISV theory to capture different dislocation types for a 3104 aluminum alloy, and [Ahmed et al. \(2005\)](#) used an ISV theory to capture the detailed history effect of rolling on a 5083 aluminum alloy. Hence, rolling was an early focus of the use of ISV theory. Issues still pertinent to rolling, however, are related to how the ISV theories can be used in the numerical frameworks (c.f., [Ziefle and Nackenhorst, 2008](#)).

Forging was also a focal point on using ISV theory in materials processing. For example, [Shiau and Fong \(1991\)](#) employed an ISV model with two hardening ISVs for hot forging of aluminum alloys that experienced different temperatures and strain rates. [Busso \(1998\)](#) examined hot forging using an ISV theory that added dynamic recrystallization and grain growth processes. The theory relied on scalar ISVs explicitly linked to intrinsic microstructural length scales, i.e. mean dislocation spacing and average grain size to describe the evolving microstructure. The formulation incorporated a material instability criterion to define the onset of recrystallization that depended on a critical mean dislocation spacing. The kinetics of grain size refinement during recrystallization and of the subsequent grain growth was controlled by the energy stored by the total dislocation density and by the grain boundary energies of the newly recrystallized grains. Clearly, these types of formulations for forging could have been used for other boundary value problems like rolling as well.

For forming, [Horstemeyer \(2000d\)](#) employed the [Bammann ISV model \(1993\)](#) to quantify and parameterize forming limits for aluminum alloys. The plasticity-damage ISV model was critical in order to capture the various localization and failure strains under different stress states. Path history effects were also elucidated by using the ISV theory.

Annealing is quite a different materials processing technique when compared to rolling, forging, and forming. The temperature dependence on the static recovery and recrystallization are key microstructural details. [Militzer et al. \(2003\)](#) needed multiple ISVs to model continuous annealing of steels and aluminum alloys used for automotive applications. The ISV model captured softening because of recovery, recrystallization, and texture, and the ISVs particularly included dislocation density, fraction recrystallized, grain size, and fraction of major texture components. A rule of mixtures was needed to reflect the combined evolving softening contributions from recovery and recrystallization.

Machining involves not only large deformations but large temperature transients and damage evolution. [Chuzhoy et al. \(2002, 2003\)](#) used the [Bammann et al. \(1993\)](#) ISV model to simulate ductile iron machining processes. [Guo et al. \(2006, 2008\)](#) employed the ISV model of [Bammann et al. \(1993\)](#), [Horstemeyer et al. \(2000\)](#) to study hard machining of different metal alloys. His results were validated with different experiments by examining the geometry of the chips.

Up to now, modeling different materials processing techniques has been performed on materials mostly made of steel and aluminum alloys. Fairly recently, magnesium has had a resurgence for application in structural components and ISV theory has been applied to magnesium as well. [Lee et al. \(2004\)](#) studied the superplastic deformation of an AZ31 magnesium alloy using ISV theory for dislocation work hardening.

Inherent within materials processing is the notion of the history of the material. Currently, only ISV theory can address the prediction of desired properties because of the ability to capture history effects.

In the previous paragraphs, we focused on materials processing related to history effects in the context of engineering solutions. However, more scientific studies related to the usage of ISV modeling and associated experimental validation

efforts have been performed. Although thoughts regarding the modeling of history effects have been prevalent, it was not until Green and Rivlin's (1957) formalism for modeling history effects (or material memory) those continuum theories addressed the issue. Although this formalism was not cast in an ISV framework, because it had not been created yet, it was a mathematical forerunner. Both small and large strain formulations have included ISVs in order to capture path history effects. For small strains, McDowell (1985a,b) employed multiple ISV kinematic hardening variables to capture cyclic plasticity responses. Many cyclic plasticity ISV models have been employed in the past. Recently, Neu et al. (2000) introduced new experimental techniques to more accurately calibrate the McDowell ISV cyclic plasticity model. Up to this time, directly experimentally measuring ISVs was virtually impossible. A strain transient dip test and the rapid load/unload test are two indirect experimental methods used to obtain an approximate measure of the evolutionary nature of the back stress for a strain rate temperature dependent solder alloy.

Some large strain history effect studies included those with changing temperatures, strain rates, and paths. For example, Wooley (1953), Buckley and Entwistle (1956), Orowan (1958) provided early Bauschinger effect experiments, which provided a basis for dislocation histories causing deformation path dependence. In terms of modeling, Follansbee and Gray (1991) employed the Kocks MTS ISV model to capture the strain rate history tests in which yield stress and work hardening behavior at strain rates in the range  $10^{-3}$ – $10^4$  s<sup>-1</sup> for copper that has been previously shock deformed at a shock pressure of 10 GPa. McDowell (1994) described the application of ISV theory for work hardening that experienced nonproportional loading, cyclic strain accumulation in the presence of mean stresses, temperature and strain rate dependence and history effects, deformation induced anisotropy at finite strain, and compressibility effects for porous metals. Employing a polycrystalline ISV plasticity model, Horstemeyer and McDowell (1995) compared non-monotonic strain path change tests results with the model and discussed the effects of texture. Later, Tanner and McDowell (1999a,b) performed a series of large strain deformation experiments on copper involving sequences of deformation path, temperature, and strain rate (quasi-static to dynamic) to modify the Bammann et al. (1993) ISV plasticity model. The history modeling-experiments included: (a) constant true strain rate tests at various temperatures, (b) load–unload–hold–reload tests at several temperatures, and (c) sequence tests, including strain rate changes, temperature changes and deformation path changes. At the same time, Miller et al. (1999), Harley et al. (1999) performed large strain Bauschinger effect tests on a stainless steel alloy. Another example was the work of Juhasz et al. (2000), who employed an ISV theory to capture shape-memory alloy stress–strain behavior under large strains. And finally, Raeisinia et al. (2006) employed ISV hardening equations to capture multistep heat treatments for an aluminum alloy.

## 7. Continuum damage mechanics

Continuum damage mechanics has been used in both the metals and polymer-based composites communities. In this section, we follow the history of the metal materials, because that is where the notion of damage started. We discuss the damage mechanics related to composites in a later section in this paper.

Kachanov (1958) first introduced the notion of damage as a reduction of the strength with an associated porosity or a void volume fraction. Rabotnov (1963) extended this work by introducing a rate equation for void growth in the context of creep. These studies were the precursors to the modern continuum damage mechanics, which is rooted in the Coleman and Gurtin (1967) formalism of ISV theory. McClintock (1968) moved the notion of rate equations for damage from creep to plasticity as he introduced a void growth rule based upon the stress triaxiality arising from the physical observations of Bridgman (1923). Later, a popular paper by Gurson (1977) laid the foundation for integration all of the governing equations into a damage framework although the evolution of damage was not explicitly related to a void growth rate equation as per the ISV rigor. Leckie and Onat (1981) developed higher order tensorial representations for damage as ISVs. Sawczuk (1984) developed the thermodynamic rate equations for creep damage after the character of Rabotnov (1963). Perzyna (1985) employed a porosity ISV into an elastoviscoplasticity theory in order to capture spallation of aluminum and copper under high rate loads. Essentially, the porosity ISV led to ductile fracture of under the dynamic conditions.

Aktaa and Schinke (1996) employed an ISV for damage that indirectly captured the effects of porosity in that damage evolution, damage under uniaxial strain controlled cyclic tests were reflected in the change of the modulus of elasticity and the decrease of the peak stress. This notion of damage in which the “effect” of the porosity operates on the elastic modulus and stress state is similar to that spirit of Gurson (1977). This approach is different than that of Chaboche (1981, 1986, 1988a,b), Lemaitre (1984, 1985), Perzyna (1985), Bammann and Aifantis (1989), Bammann et al. (1993) who included a direct rate equation for porosity growth that operated on the thermodynamic potential.

For example, Bammann et al. (1993) employed the Cocks and Ashby (1980) creep void growth rule into the ISV formalism with large deformation kinematics. Voyiadjis et al. (1992, 1995, 1996, 1999, 2001) advanced the original higher rank tensorial ISV damage by including kinematics, kinetics, and thermodynamics for the development of the rate equations. Kawai (1995) extended the Kachanov (1958) and Rabotnov (1963) creep constitutive model into the irreversible thermodynamics for ISV theory; here, Kawai (1995) employed thermodynamic potentials with free energy and dissipation energy functions that defined the hardening and damage variables. The coupled damage kinematic hardening model was developed in the invariant form on the basis of the Malinin–Khadjinsky model. The evolution equation of the hardening variable followed the Bailey–Orowan format, which included the effects of isotropic damage. Kawai (1995) also included an isotropic hardening model with the consideration of damage as well. Radayev (1996) extended the Kachanov (1958) and Rabotnov (1963)

equations directly into a thermodynamic ISV formalism with an anisotropic damage growth model in its canonical variant. Marin and McDowell (1996) evaluated several different elastoviscoplastic ISV damage models that incorporated porosity in the context of associative and non-associative numerical frameworks. They illustrated the usages of the ISV damage models by applying the Bammann et al. (1993) formalism to several complex boundary value problems within the context of finite element analysis. Laemmer and Tsakmakis (2000) examined three different ISV plasticity-damage models that included one isotropic hardening ISV, one kinematic ISV, and one damage ISV similar to the Bammann et al. (1993) framework and showed the differences in the models for small and large strains. In Horstemeyer et al. (2000e), different ISV rate equations were introduced as separate void nucleation, void growth, and void coalescence equations were added to the Bammann et al. (1993) ISV formalism. Later, Horstemeyer and Wang (2003) argued that the generalized plasticity-damage framework of Horstemeyer et al. (2000e) could be applied to different metal alloys and different materials processing methods because microstructural quantities such as pore size, particle size, grain size, and their distributions could explicitly be placed into the ISV rate equations. Later, Hammi et al. (2003, 2004, 2007) extended the work of Bammann et al. (1993), Horstemeyer et al. (2000e, 2003) by introducing higher order tensorial rank tensors to represent the plasticity and damage evolution as represented by separate rate equations for void nucleation, growth, and coalescence. Lorentz and Benallal (2005) developed an ISV formulation for damage of brittle materials but introduced a gradient theory on the damage to address localization as well as damage. Later, Voyiadjis and Dorgan (2007), Voyiadjis and Deliktas (2009) showed the use of higher order rank ISV tensors for anisotropic plasticity and damage modeling of metals and for nonlocal damage. Besson (2009) recently employed an ISV formulation in the CMD context to capture the effects of creep and he also (Besson 2010) recently reviewed some of the continuum damage models related to local and nonlocal constitutive models.

In terms of damage and fracture, Griffith (1921) found a relation between the crack length and the stress intensity factor in the absence of microstructural features, because long crack growth is driven by mechanics. However, before this time, Roberts-Austen (1888) performed a set of experiments that showed the tensile strength of gold having a strong dependence of the impurity size within a material. Fairly recently, McClintock (1968) determined the void growth rates as a function of the void size. Void/crack nucleation was determined by various aspects of the second phase particle size distribution by Gangalee and Gurland (1967). Needleman (1996) determined the scaling length associated with a void sheet as a function of void spacing and diameter. Horstemeyer et al. (2000b,c), Potirniche et al. (2006a,b,c,d) determined the nearest neighbor distance as a length scale parameter for an ISV rate equation to capture void coalescence for different metals that was experimentally validated by Jones et al. (2007). Void nucleation ISV rate equations were developed by Horstemeyer and Gokhale (1999) that was motivated from multiscale modeling (Horstemeyer et al., 2003b). It is clear that whether damage mechanics or fracture mechanics is employed, the length scale of interest is important to model this type of inelastic behavior. Furthermore, since changes do occur in the void nucleation, growth, and coalescence, ISV rate equations are warranted for modeling the history effects.

## 8. Multiscale modeling

Inherent within ISV theory are the different mechanisms at different length scales within the material. To decide on the pertinent length scale feature of importance, one must consider that in modern solid mechanics, continuum theories are driven by the conservation laws (mass, momentum, and energy); however, there are too many unknowns than the number of equations, so constitutive relations (sometimes erroneously called “laws”) are required to solve the set of differential equations for finite element or finite difference analysis (most modern solid mechanics tools employ finite element analysis). When developing a multiscale modeling methodology for ISV constitutive relations, the kinetics, kinematics, and thermodynamics need to be consistent in the formulation. There are also certain classical postulates in continuum theory that guide the development of the constitutive theory (objectivity, physical admissibility, equipresence, and locality). Multiscale modeling has been driven by the physical admissibility postulate even at the expense of the postulates of equipresence and locality. Physical admissibility essentially means identifying the physical mechanism or discrete microstructural feature at the particular length scale that is a root source of the phenomenological behavior.

Two different general multiscale methodologies exist starting from the solid mechanics continuum theory paradigm: hierarchical and concurrent. Reviews have been given on these methods by Phillips (2001), Liu et al. (2006b), Fish (2006), de Pablo and Curtin (2007). The key difference between the hierarchical and concurrent methods is the bridging methodology. In concurrent methods, the bridging methodology is numerical or computational in nature. In the hierarchical methods, numerical techniques are independently run at disparate length scales. Then, a bridging methodology such as statistical analysis methods, homogenization techniques, or optimization methods can be used to distinguish the pertinent cause-effect relations at the lower scale to determine the relevant effects for the next higher scale.

One effective hierarchical method for multiscale bridging is the use of thermodynamically constrained internal state variables (ISVs) that can be physically based upon microstructure–property relations. It is a top–down approach, meaning the ISVs exist at the macroscale but reach down to various subscales to receive pertinent information. Essentially, the subscale simulations can be used to determine the appropriate ISV.

A good example of a bad usage of a variable is using OSVs for ISVs. For example, strain is an OSV, but has been used to represent effects of dislocations at lower length scales (Fleck et al., 1994). Horstemeyer (2003) examined FCC nickel undergoing simple shear by using three different numerical frameworks formulated at three different size scales. The three

frameworks included embedded atom method potentials used in molecular dynamics simulations, crystal plasticity used in finite element simulations, and a macroscale internal state variable formulation used in finite element simulations. The three results gave the same strain responses indicating that self-similar scale invariance is a true identity for the observable state variable of strain. Alternatively, the stress state increased as the length scale decreased because of the local dislocation nucleation, motion, and interaction indicating that the effects of dislocations represent a very good internal state variable and in particular one with a length scale. Bammann (2001) laid out the ISV thermodynamics with a natural length scale parameter imbedded within the ISV dislocation density and not the OSV strain.

## 9. Multiphase Materials

ISV theory has found its way into multiphase materials, mainly the solid–solid types. Tanaka and Nagaki (1982) were probably the first to use an ISV continuum description for thermoplastic materials in the process of solid–solid phase transitions. Three ISVs were employed: two ISVs for the crystallographic structural change during the plastic deformation, and a set of scalar ISVs to describe the extent of the phase transitions. Applying Edelen's decomposition theorem, the plastic quantities were determined from the dissipation potential, while the elastic quantities were specified by the internal energy. Bammann et al. (1995) extended their earlier elastoviscoplastic ISV theory (Bammann et al., 1993) by adding multiple phases with an interaction term in a mixture theory for heat treatment of steel alloys. Bo and Lagoudas (1999) introduced a set of ISVs to represent martensitic phase transformations, a transformation strain-like quantity, a backstress for kinematic hardening, and a drag stress for isotropic hardening. They applied this multiphase ISV theory to a Shape Memory Alloys (SMAs) to capture the microstructure and associated mechanical property history effects. Later, Lusk et al. (2003) showed that the fundamental thermophysical functions can be determined from the kinematics of multiphases by using an ISV model for austenite decomposition. The key idea here was that the kinetic parameters within the ISVs were optimized so as to match dilatometry data without the need to heuristically back out any phase fraction data prior to fitting. Other ISV models related to SMAs include those of Lim and McDowell (1995, 1999, 2002), Luig and Bruhns (2008),

In a different usage of ISV theory, Abriata and Laughlin (2004) employed ISVs in the context of multiphase inelasticity where phase stability, phase boundaries, and the related phase diagrams at particularly low temperatures were studied in the light of the restrictions imposed by the Third Law of Thermodynamics. The Third Law of Thermodynamics is a statistical law of nature regarding entropy and the impossibility of reaching a temperature of absolute zero. Essentially, when a system approaches absolute zero, all processes cease and the entropy of the system approaches a minimum. For ordinary materials (most engineering materials have multiple phases) the equilibrium state of 0 K should satisfy the two conditions that its energy and entropy are at their lowest possible values as permitted by the rate constraints imposed on their OSVs and ISVs. As such, the free ISVs (such as the equilibrium compositions of coexisting phases) must be such that the rates of change of their equilibrium values as a function of temperature are zero at 0 K.

In the literature, some experimental results of polycrystalline NiTi shape memory alloys reveal a strong change in temperature occurring in the linear elastic strain range owing to the evolution of martensite. To consider this effect in material models, Luig and Bruhns (2008) introduced a tensorial ISV for the description of the phase transformation along with a suitable approach for the inelastic strain rates resulting from the formation of martensite. For the evolution of ISV phase transformations two issues are considered: first, the scalar mass fraction of martensite, and second, the orientation of the martensite variants.

## 10. Polymers

Although metals have enjoyed a rich history of ISV usage, the application to polymers has not been as prevalent. The complexities of polymers are different than metals (c.f., Argon, 1973), but the methodology of embedding mechanisms into the ISV framework that is constrained by thermodynamics is the same. For example, Arruda et al. (1993a,b) developed an ISV formulation for evolving anisotropic viscoelastic polymers based upon the previous viscoplastic formulations for metals. This work was based on the fundamental work of mechanism modeling by Parks et al. (1985), Boyce et al. (1988). During processing glassy polymers produce highly anisotropic polymer components as a result of the massive reorientation of molecular chains during the large strain deformations. Using material properties from initially isotropic material, simulations were shown to capture the important aspects of the large strain anisotropic response including flow strengths, strain hardening characteristics, cross-sectional deformation patterns, and limiting extensibilities.

Later, others developed ISV theories for polymers. Schapery (1999) developed an ISV formalism for nonequilibrium thermodynamics, strain rate sensitive, viscoelastic fracture mechanics that accounted for effects of viscoelasticity, viscoplasticity, growing damage and aging. Within this research effort, Schapery (1999) analyzed the isotropic and anisotropic aspects of the ISV formalism. Yoon and Allen (1999) introduced a cohesive fracture model into an ISV formulation for nonlinear viscoelasticity materials. Wei and Chen (2003) proposed an ISV model that extended the network theory of rubber elasticity with viscosity. Based on the thermodynamics of Anand and Gurtin (2003), Gearing and Anand (2004) used ISVs to represent crazing and damage for polymers and later Anand and Ames (2006) added ISVs to represent other mechanisms as inelastic dissipative mechanisms for viscoelastic polymers. Recently, Anand et al. (2009) coupled the temperature effects with the previous works and then employed the ISV modeling framework on several polymer systems to illustrate the robustness of the model.

Polymers exhibit a strong history effect and maybe moreso than metal alloys because of their rate sensitivity. A good example that demonstrated this phenomena was the work of Liu et al. (2006a), who experimented with shape memory polymers (SMPs) and developed an ISV theory to capture the effects. Up to this point, little progress had been made on modeling the thermomechanical coupling of SMPs. In this study, the thermomechanics of shape storage and recovery of an epoxy resin was systematically investigated for small strains (within  $\pm 10\%$ ) in uniaxial tension and uniaxial compression. After initial pre-deformation at a high temperature, the strain was held constant for shape storage while the stress evolution was monitored. Three cases of heated recovery were selected: unconstrained free strain recovery, stress recovery under full constraint at the pre-deformation strain level (no low temperature unloading), and stress recovery under full constraint at a strain level fixed at a low temperature (low temperature unloading). The free strain recovery result indicated that the polymer fully recovered to the original shape when reheated above its glass transition temperature ( $T_g$ ). Due to the high stiffness in the glassy state ( $T$  less than or equal  $T_g$ ), the evolution of the stress is strongly influenced by thermal expansion of the polymer. The relationship between the final recoverable stress and strain was governed by the stress–strain response of the polymer above  $T_g$ . The model quantified the storage and release of the entropic deformation during thermomechanical processes. The fraction of the material freezing a temporary entropy state is a function of temperature, which can be determined by fitting the free strain recovery response. A free energy function for the model was formulated to ensure thermodynamic consistency. The model captured differences in the tensile and compressive recovery responses caused by thermal expansion. The model was also used to explore strain and stress recovery responses under various flexible external constraints that would be encountered in applications of SMPs.

In another study, Gilat et al. (2007) applied an ISV theory to resin epoxy undergoing varying strain rates including high rates under Hopkinson bar loading conditions. They also analyzed the stress state dependence of these resins by employing tensile and shear loading conditions and showed that the ISV formulation was robust enough to capture the results. Also in 2007, Näser et al. (2007) studied the large strain history effects of polymer materials using an ISV formalism.

Recently, Ghorbel (2008), Cantournet et al. (2009) modified a viscoplastic ISV formulation to use for viscoelastic polymers by changing the yield function to include the first three invariants of stress to include pressure dependence and strong deviatoric interactions. At the same time, Cantournet et al. (2009) developed an ISV formulation to capture the phenomenological effects in filled elastomers based upon the work of Arruda and Boyce (1993b) where friction evolution rules were employed to capture effects arising from sliding of chains-on-chains and chains-on-filler particles.

## 11. Composites

The terminology of composites in materials science has been generalized to represent any engineering material whether it is a metal with various constituent phases or polymers with particles. However, the major paradigm for composites is really related to polymer-based composites, for the most part, with glass or carbon based fibers as applied for structural and mechanical components. It is this context by which we discuss the use of ISV theory in composites. Of course, the issue that these composites bring is the initial anisotropy of the properties and the subsequent anisotropic damage evolution.

Krajcinovic et al. (1981, 1983, 1984) probably was the first to introduce the term continuum damage mechanics (CDM) as a branch of continuum solid mechanics characterized by an ISV, representing the distribution of microcracks locally. In particular, he described the internal state of the material by the density (which changes with defects), defects distribution, and type of defects and asserted that these can be changed only at the expense of externally supplied energy. The model was developed within the framework of the general thermodynamics theory as the damage law was derived from the dissipation potential in conjunction with the orthogonality principle. The dissipation potential was shown to exist in the space of conjugate thermodynamic forces related to the stress intensity factors. Both brittle and ductile materials were considered within the framework of the small deformation theory and the time-independent processes thus leading to the basis for the composites work using ISV theory.

Talreja (1987, 1991, 1993, 1997) based on the work of Coleman and Gurtin (1967) employed damage ISV equations by a set of ordinary differential equations describing the temporal evolution of polymer-based laminated composites. Each ISV represented a different damage mode as were represented by second rank tensors thus allowing for the anisotropy. The evolution equations were restricted by the material symmetry in addition to the thermodynamical restrictions of Coleman and Gurtin (1967). Experimental data showed good correlations to the model. Fu and Wang (2004) employed Talreja's ISV framework to study buckling of composites.

At the same time as Talreja's studies, Allen et al. (1987) developed ISV composites models to characterize damage by a set of second-order tensor valued internal state variables that represented locally averaged measures of specific damage states such as matrix cracks, fiber-matrix debonding, interlaminar cracking, or any other damage state similar to Talreja. Harris et al. (1989) extended the work of Allen et al. (1987) by focusing on experiments of matrix cracks and delaminations for graphite-epoxy laminated composites. The ISVs are defined as the local volume average of the relative crack face displacements.

Li et al. (1992) focused on using an ISV theory for matrix cracking in a fiber reinforced plastic. The matrix cracks were assumed to be an array of parallel cracks along fibers in the plies, and the average measurement of the damage by the ISV. In the same year, Sanders et al. (1992) used nondestructive evaluation methods to quantify the damage as represented by ISVs for fiber reinforced composites. They also examined via the experiments model sensitivity parameters and the experimental results matched the ISV theory fairly well.

Yang and Engblom (1995) cast an analytical sub-laminate ISV model of intralaminar cracking to represent a particular ply or sub-set of adjacent plies (layers) of equal orientation. The formulation was implemented into a finite element code so that variations of material properties evolving from intralaminar cracks arose.

Kanagawa et al. (1996) described anisotropic damage states in fiber reinforced plastic laminates with second rank damage tensors that were based on the strain equivalence and strain energy equivalence principles.

Lacy et al. (1997) performed micromechanical simulations to motivate ISV phenomenological damage theories related to microcracking. Up to this point, continuum level composite laminate ISV theory did not explicitly account for distributions of microcracks in a representative volume element (RVE). Lacy et al. (1997) showed that while the distribution and interaction of damage entities within the RVE minimally affect the effective moduli, it significantly affects the damage progression and failure at the macroscale. Their conclusion was that damage evolution rates cannot be described adequately by such purely phenomenological theories because of their inability to account for interactions between damage entities in an arbitrary distribution.

Park and Schapery (1997), Schapery (1999) developed a thermomechanical model in which the ISV damage evolution equations were validated by experiments of a viscoelastic filled elastomer.

Recently, Mohite and Upadhyay (2008) employed a two-length scale composites damage ISV model in which the subscale simulations provided key damage progression data for the ISV phenomenological behavior in a fiber reinforced composite.

Some work has been conducted in placing fiber reinforcement into a metal matrix, but only minimal work in ISV has been employed. For example, Kawai (1995), Kawai and Morishita (1996) employed ISVs for creep deformation and damage of uni-directional fiber-reinforced metal matrix composites. The model was based on the thermodynamics of Coleman and Gurtin (1967). A damage-coupled kinematic hardening model for transversely isotropic materials was first formulated as an invariant form on the basis of the Malinán and Khadjinsky (1972) anisotropic creep model.

## 12. Biomaterials

Biomaterials can be thought of as a polymer based system or a composite since all of the organ's base structure includes multiple materials. Little work has been accomplished in the realm of using ISV models for finite element analysis of the human body. However, a few studies have indeed been performed.

For bone, Fondrk et al. (1999) introduced a damage model that was developed using two ISVs. One ISV was a damage parameter that represented the loss of stiffness, and a rule for the evolution of this ISV was defined based on previously observed creep behavior. The second ISV represented the inelastic strain due to viscosity and internal friction.

For soft tissues, Engelbrecht et al. (2000) formalized an ISV theory that described the processes of nonlinear deformation. They focused the ISVs on the sliding of molecules and ion concentrations. An application of the ISV model was used to correlate with muscle experiments.

For general inorganic materials, Herrmann (2007) developed an ISV theory based on conventional thermodynamics of irreversible processes, where the concept of a local thermodynamic state plays a prominent role. An elastic body prone to damage was regarded as a thermodynamic system characterized by a set of ISVs that can be defined in both equilibrium and nonequilibrium states and assigned approximately the same values in both the physical space and the abstract Gibbsian phase space.

## 13. Particulate materials (geomaterials and powder metals)

Particulate materials include powder metals and geomaterials such as sand, soil, snow, and other such naturally occurring materials. To model these materials with ISV theory, the mathematical formalism is similar but because of the pressure dependence, the first invariant of the stress tensor needs to be employed.

Before an ISV formulation was applied to geomaterials, Drucker et al. (1957) formulated the CAP model for particulate materials that experience plasticity. Later, Dorris and Nemat-Nasser (1980), Nemat-Nasser and Shokooh (1980) developed plasticity formulations for particulate materials under compression raising the point of modeling friction. From this background, Hansen and Brown (1988) first proposed an ISV theory for a particulate material and applied the model to snow. Later, Sunder and Wu (1989, 1990) used two ISVs for isotropic and kinematic hardening for capture ice effects. Aubertin et al. (1991) developed an ISV model for application to the creep response of rock salt. Emeriault and Cambou (1996) developed a nonlinear elasticity model with ISV that was derived from a microscopic Hertz–Mindlin elastic contact law using a homogenization technique for granular materials. Abe (1997) developed an ISV elastoviscoplastic constitutive model to predict the one-dimensional consolidation behavior of natural soft clay deposits. Aubertin et al. (1999a,b) extended the previous ISV model (Aubertin et al., 1991) for inelastic flow of alkali halides and various rocks that behaved fully plastically showing strong rate and history dependencies and anisotropic hardening. Li and Dafalias (2000) introduced an ISV theory for loose and dense sands in which the dissipative mechanism was tied to the pressure dependence. Collins and Kelly (2002) developed an ISV theory that was able to predict non-associated flow rules, contractive behavior, pre-peak failure instabilities, and ultimate state lines. At the same time Cheng and Dusseault (2002) presented a continuum damage mechanics constitutive model for brittle geomaterials based on irreversible thermodynamics with ISVs. Damage was incorporated by a porosity ISV. The thermodynamic

basis, free energy function, damage evolution equation, and damage-induced inelastic compliance were derived and the model showed that damage caused strain softening, positive dilatancy, and a decrease of the material stiffness. [Wei and Dewoolkar \(2006\)](#) developed a thermodynamically consistent framework proposed for modeling the hysteresis of capillarity in partially saturated porous media. Here, the capillary hysteresis is viewed as an intrinsic dissipation mechanism and modeled by an ISV. In relation to high rate phenomena of particles, [Austin et al. \(2006\)](#) employed an ISV scheme in Eulerian and Lagrangian numerical schemes to study the responses of different metals. Later, [Cai and Li \(2007\)](#) applied an ISV theory with a pressure dependence for sand modeling. Recently, [Kohler and Hofstetter \(2008\)](#) extended a cap model with two ISVs to capture the material behavior of partially saturated soils, sands, and silts. Each ISV represented a matrix section to induce plasticity, and the yield surface comprised a shear failure surface and an ISV hardening cap surface for non-associated flow.

For powder metals, the CAP model ([Drucker et al., 1957](#)) had been the precursor to ISV modeling of the inelastic behavior. [Dimaggio and Sandler \(1971\)](#) included the evolution of density in the CAP framework but did not include it in the context of an ISV theory. [McMeeking \(1992\)](#) was the first to employ ISV theory to powder metals for sintering and hot and cold compaction. He employed multiple ISVs to capture behavior for dislocation creep, diffusion creep, sintering, and density (porosity). [Fleck \(1995\)](#) developed an ISV constitutive model for cold compaction of powders under general multi-axial loading. Densification occurred by plastic deformation at the isolated contacts between particles. The yield surface shape was found to be sensitive to the cohesive strength between particles and to be less sensitive to the interparticle friction. An internal state variable model was used to describe the evolution of anisotropy under general loading. Later, [Hilinski et al. \(1996\)](#) studied the compaction of aluminum powders using one ISV in a finite element simulation. [Li et al. \(1998\)](#) employed an ISV model for pressure-dependent metals to distinguish between tension and compression.

#### 14. Multi-physics

Fairly recently, ISV theory has been introduced into multi-physics problems since the coupling of different physical entities and mechanisms can be coupled within the framework. [Maugin \(1993, 1994\)](#) for example, laid out a general theory of nonequilibrium thermodynamics offering a deviation from the classical theory. The identification of ISVs with order parameters of phase transition theory and their differences with extended thermodynamics are presented. [Maugin \(1997\)](#) extended the [Maugin \(1993, 1994\)](#) theory for a unified multiphysics thermomechanical framework of which required additional ISVs and their associated gradients (weak nonlocality). This included both the case of additional degrees of freedom carrying their own inertia and the case of diffusive ISVs. In view of practical applications to fracture and propagation of phase-transition fronts, special attention was paid to the construction and immediate consequences of the equations of balance of canonical momentum (on the material manifold) and energy at regular points and at jump discontinuities. The theory was shown to apply to thermoelastic conductors (e.g., shape-memory alloys) and elastic ferromagnets in which both spin inertia and ferromagnetic exchange forces (magnetic ordering) were considered. [Narayanan et al. \(2003\)](#) modeled the thermoferroelastic hysteresis of piezoceramic materials under large mechanical loading by using ISVs that were associated with a statistical description of various microstructures. [Francaviglia et al. \(2004\)](#) used the [Maugin et al. \(1994, 1997\)](#) ISV model for thermoelastic materials. The polarization together with its space gradient was assumed as ISVs expressed in a relaxation law driven by external and internal electric fields. For other materials, [Mehling et al. \(2005, 2006, 2007\)](#) employed an ISV theory for application to ferroelectric polycrystalline ceramics (like PZT or Barium Titanate), which experienced texture and an anisotropic polarization state. One ISV was a second-order texture tensor, determining a simple orientation distribution function (ODF) for the axes of the crystal unit cells. The second one was a vector of relative irreversible polarization. For nonlinear irreversible processes, a switching function and associated rate equations were used to satisfy the principle of maximum ferroelectric dissipation. A saturation state as defined by the ISVs was modeled by the use of energy-barrier functions in the electric enthalpy density function.

For a different multi-physics problem, [Wang and Xiao \(2001\)](#) developed an ISV theory with microstructural effects from electrically resistive suspensions, which are essentially fine particles with a high dielectric constant in a supporting fluid. Under the action of the electric field, the polarized particles aggregate together to form the chain-like structures along the direction of the electric field. As the size and orientation of the particle aggregates are volatile, and they adjust according to the applied electric field and strain rate, the energy conservation equation, energy dissipation, and the force equilibrium equations were developed to quantify the orientation and size of the aggregates.

[Kiefer et al. \(2005\)](#) developed an ISV theory to solve a magnetically induced martensitic variant reorientation process under applied mechanical load in magnetic shape memory alloys (MSMAs). The material shows a nonlinear and hysteretic macroscopic strain response under variable applied magnetic field in the presence of stress, also known as the magnetic shape memory effect (MSME). A thermodynamically consistent phenomenological constitutive model was derived capturing this effect using ISVs, which were chosen based on the crystallographic and magnetic microstructure.

One final multi-physics example of using ISV theory is that from [Chen \(2007\)](#), who introduced an ISVs to couple hygrothermo-viscoelastic effects into a fracture theory for quasi-static and dynamic crack propagation. Viscoelastic materials were subjected to combined mechanical loading and hygrothermal exposure. The Helmholtz free energy was taken to be a function of the histories of the normal OSVs and the fluid concentration with the crack parameter being introduced as an ISV.

## 15. Structure–property relations

Ashby (1992) described the general approach of trying to incorporate lower length scale mechanisms into a material modeling framework to address the history effects arising from the processing and engineering properties of materials. A flowchart for model development was presented with the idea of an ISV theory capturing the important microstructural features. Earlier, Swearingen and Holbrook (1985) discussed the difficulties of imbedding microstructural details into the ISVs. In terms of viscoplasticity for metal deformation they purported that a universal model was possible that may be constructed from microstructural information and physical laws. A little later, Stone (1991) developed an ISV model for creep in which the plastic flow properties depended upon the diameters of subgrains generated during deformation. The subgrain diameters incurred a self-similar scaling distribution such that an internal state variable arose for the dislocation plasticity.

At the same time from a mechanics perspective, Onat (1991) laid out the theoretical result that the observed mechanical behavior of a material can be represented by ISV differential rate equations and that these ISVs are even rank irreducible tensors. On the other hand microscopic observations of internal structure of a material produce functions that are defined on 'curved' objects such as the unit sphere of directions or the set of distinct orientations of a cube. Such representations of the functions give rise to Fourier coefficients that are also irreducible tensors. The tensorial ISVs were related to these tensorial Fourier coefficients. A major problem of mechanics of materials is to develop methods that enable one, for a given material and for a given purpose, to extract tensorial ISVs and the associated rules for their evolution from the knowledge obtained from the particular structure–property relationships of that material.

It was not until Horstemeyer et al. (2000e) that a complete theory using ISV hardening equations and porosity evolution equations for damage were incorporated into a large deformation kinematic and thermodynamic framework that admitted explicit structure–property relations. Hence, a finite element simulation could have different grain sizes, particle sizes, and volume fractions, pore sizes, and volume fractions within each element so that heterogeneous materials was represented within the whole mesh. Horstemeyer et al. (2000), based upon the Bammann et al. (1993) plasticity and damage philosophy, added separate ISV equations for pore nucleation, growth, and coalescence and included directly into the equations the grain size, particle size, particle volume fraction, pore volume fraction, and nearest neighbor distances of the particles and pores. This allowed heterogeneous distributions of microstructures throughout a finite element mesh to be used for complex engineering boundary value problems. In Horstemeyer et al. (2002), which was based upon a multiscale modeling strategy, the ISV theory showed that standard homogeneous distributions of microstructure and porosity, which is the classical manner of performing finite element analysis, can lead to erroneous results and conclusions. Hence, the advantage of using ISV theories that admit microstructural details for finite element analysis is to get much more accurate answers.

After Horstemeyer's work, others started to embed microstructural features into ISV formulations. Obataya et al. (2001) included two ISVs: one related to dislocation density and the other related to evolving ratio of the grains with activating slip systems greater than five to the total grains. Spearot et al. (2004) proposed an ISV formulation for a cohesive law to characterize fracture. They developed a continuum interface separation constitutive law that was motivated by molecular dynamics (MD) simulations which accounted for the influence of atomic structure and imperfections on interface separation or fracture. The proposed interface ISVs accounted for geometry, composition, defect density, and damage within the interface region. Shenoy et al. (2008) developed a rate dependent, microstructure-sensitive crystal plasticity model formulated for correlating the mechanical behavior of a polycrystalline Ni-base superalloy IN 100. This model has the capability to capture first order effects on the stress–strain response due to (a) grain size (b)  $\gamma$  prime precipitate size distribution, and (c)  $\gamma$  prime precipitate volume fraction using ISVs. Tjiptowidjojo et al. (2009) developed an artificial neural network to correlate the material constants of an ISV cyclic viscoplasticity model with these microstructural attributes using a combination of limited experiments augmented by polycrystal plasticity calculations performed on virtual microstructures within an experimentally characterized range.

## 16. Design optimization under uncertainty

One of the main purposes of employing an ISV theory that can admit microstructural heterogeneities within a finite element analysis is to design new components and structures in an optimal manner. Historical designs employ trial-and-error methods and even with the use of a simulation-based design methodology, predictions have been off mainly because simulations did not have the structure–property identities. Now that the ISV theories can admit the structure–property relations, design optimization is plausible with different models and codes (c.f., Foerch et al., 1997). Horstemeyer et al. (2002), Horstemeyer and Wang (2003) showed that an automotive control arm, by employing the Horstemeyer et al. (2000) ISV theory with microstructure, could be optimized. In that case, a Cadillac control arm's weight was reduced 25% and the cost was reduced 12%. However, the load bearing capacity increased 50% and the fatigue life increased 100%. The point is although the Cadillac control arm worked before this analysis, it was not optimized. Given the state of simulation based design with the incorporation of microstructural details, the design paradigm can now change and newer more robust lightweight designs are plausible. For example, Solanki et al. (2007) employed a formal optimization algorithm for this application using the ISV formalism. Others have recently employed optimization under uncertainty with ISVs as well (c.f., To et al., 2008; Yin et al., 2008, 2009).

## 17. Summary

The watershed article of Coleman and Gurtin (1967) laid the foundation for ISV theory to be implemented into the finite element analysis discipline. With this advent, more accurate designs and analysis became feasible over the past 40 years for different materials. Many different ISV models were employed for the unified-creep-plasticity theories that were used for metals. Later, ISV theory was applied to polymer materials, both biological and synthetic, and to multiphase materials like polymer-based composites. The greatest impact for ISV theory has yet to be realized, because now new design of materials and structures is admissible because of the structure–property capabilities of the ISV theories. For predictive science to be used for a broader range design and manufacturing corporations, an ability to capture the history of the material in terms of the structure–property relations and clearly ISV theory can address this issue. It has been the dream of manufacturers to use models to help optimize the material during its whole processing history with inclusion of costs. ISV theory has the potential for manufacturers to realize this dream because of the inclusion of the history effects and its implementation into common engineering practice codes.

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