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What is This?

A Finite Strain Plastic-damage Model for High Velocity Impact using Combined Viscosity and Gradient Localization Limiters: Part I – Theoretical Formulation

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ABSTRACT: During dynamic loading processes, large inelastic deformation associated with high strain rates leads, for a broad class of ductile metals, to degradation and failure by strain localization. However, as soon as material failure dominates a deformation process, the material increasingly displays strain softening and the finite element computations are considerably affected by the mesh size and alignment. This gives rise to a non-physical description of the localized regions. This article presents a theoretical framework to solve this problem with the aid of nonlocal gradient-enhanced theory coupled to viscoinelasticity. Constitutive equations for anisotropic thermoviscodamage (rate-dependent damage) mechanism coupled with thermo-hypoelasto-viscoplastic deformation are developed in this work within the framework of thermodynamic laws, nonlinear continuum mechanics, and nonlocal continua. Explicit and implicit microstructural length-scale measures, which preserve the well-posedness of the differential equations, are introduced through the use of the viscosity and gradient localization limiters. The gradientenhanced theory that incorporates macroscale interstate variables and their highorder gradients is developed here to describe the change in the internal structure and to investigate the size effect of statistical inhomogeneity of the evolution related plasticity and damage. The gradients are introduced in the hardening internal state variables and are considered dependent on their local counterparts. The derived microdamage constitutive model is destined to be applied in the context of high velocity impact and penetration damage mechanics. The theoretical framework presented in this article can be considered as a feasible thermodynamic approach that enables to derive various gradient (visco) plasticity/(visco) damage theories

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by introducing simplifying assumptions. Besides the clear physical significance of the proposed framework, it also defines a very convenient context for the efficient numerical integration of the resulting constitutive equations. This aspect is explored in Part II of this work and the application of the framework proposed herein to the numerical simulation of high velocity impacts on metal plates.

KEY WORDS: nonlocal theory, anisotropic damage, viscoplasticity, viscodamage, gradient theory, impact damage.

INTRODUCTION

STRUCTURES ARE GENERALLY subjected to impact loading, which often brings failures and serious damage in their components. The September 11th attack demonstrated the response of tall steel buildings to the impact of a fast moving airplane. Millions of terrified spectators around the world watched as the Boeing 767 moving with a cruising speed of 240 m/s (500 mph), hit the exterior wall of the World Trade Center, cut through it, and disappeared in the smoky cavity. How was it possible that the relatively weak, light, and airy airframe damaged the apparently heavy lattice of high strength steel columns?

Under high-strain rate loading a type of shear banding occurs due to a rapid local heating resulting from the intense inelastic shear deformations and propagation of shock waves. The presence of material or geometrical imperfections or the evolution of heterogeneous distribution of microdefects may trigger the formation of shear bands (Zbib and Aifantis, 1988). Further, the evolution of elastic-viscoinelastic waves due to impact loading may lead to the localization phenomena in solids (Glema et al., 2000). The failure of the structure can, therefore, occur as a result of a strain localization attributed to an inelastic instability implied by microdamage, wave reflections, and/or thermal softening during inelastic flow and damage growth processes.

Many researchers have investigated the material failure mechanism during high velocity impact conditions with the ultimate goal of designing better resistance for different structures (e.g., Johnson and Cook, 1985; Curran et al., 1987; Steinberg and Lund, 1989; Bammann et al., 1990; Zukas, 1990; Zhou et al., 1996; Sierakowski, 1997; Hou et al., 2000; Naboulsi and Palazotto, 2000; Borvik et al., 2002; Li et al., 2002). Moreover, many constitutive models that consider elastic-viscoinelastic deformation at very high strain-rates have been proposed and employed to model high velocity impact phenomena (e.g., Steinberg et al., 1980; Johnson and Cook, 1985; Zerilli and Armstrong, 1987; Steinberg and Lund, 1989; Bammann et al., 1990; Eftis et al., 2003; Voyiadjis and Abed, 2005).

It is noted that none of these constitutive models address the problem of describing high shock compression and subsequent material degradation and failure in which the latter is expressed as an evolving microflaw having a damage rate determined from micromechanical analysis. Moreover, these models cannot consider the actual sizes, shapes, and orientations of the individual microvoids and microcracks, which may have a predominant influence on the mechanical response of the material. This work recognizes the need for a micromechanical damage model that takes into account the microscopic interactions between material points (i.e., takes into account the influence of an internal state variable at a point on its neighborhood) in the simulation of metal impact problems.

The inelastic material behavior of engineering materials may be attributed to two distinct material mechanical processes: plasticity and/or damage. Plasticity or viscoplasticity (rate-dependent plasticity) theories, by themselves, are insufficient for modeling the deformation of metallic materials since both damage (microcracks and microvoids) and plasticity (dislocations) are present in their microstructure. A constitutive model should address equally the two distinct physical modes of irreversible changes and should satisfy the basic postulates of mechanics and thermodynamics. A multidissipative model that accounts for both the material plasticity and damage is necessary (e.g., Chow and Wang, 1987; Murakami et al., 1998; Abu Al-Rub and Voyiadjis, 2003). As the plasticity or viscoplasticity and damage or viscodamage (rate-dependent damage or creep) defects localize over narrow regions of the continuum, the characteristic length-scale governing the variations of those defects and their average interactions over multiple length-scales falls far below the scale of the local state variables of (visco) plasticity and (visco) damage used to describe the response of the continuum. This leads to the loss of the statistical homogeneity in the representative volume element (RVE); in such a way that all the macroscopic response functions of interest (e.g., the Helmholtz free energy, Ψ ; the dissipation potential, Π ; the Cauchy stress tensor, σ ; the small strain tensor, ε ; the stiffness tensor; C, etc.) are sensitive to the distribution, size, and orientation of the mesostructural and macrostructural defects within the RVE (see Figure 1). For example, dislocation interactions are observed on a mesolevel with a length-scale of 0.1-10 µm affecting strongly the material behavior on the macrolevel with a length-scale of >100 µm (Abu Al-Rub and Voyiadjis, 2004). Therefore, there is a need for models that abandon the assumption that the stress at a given point is uniquely determined by the history of strain and temperature at this point only (locality). This raises the need for incorporation of material length-scale measures in the constitutive description of the material mechanical behavior.

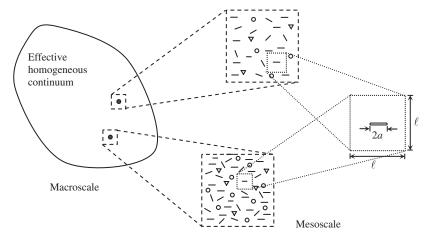


Figure 1. Macroscopic and mesoscopic observation scales: conceptual representation of the nonlocality.

The use of a classical rate-independent theory or a rate-independent local theory, which does not possess an intrinsic length-scale, leads to numerical stability problems, such as the inherent discretization dependence, particularly, in problems exhibiting strain localization phenomena (for more details see Pamin, 1994). This is clearly an undesirable state of affairs and stems from the character of the continuum equations. This drawback in the classical inelasticity arises from the fact that they do not possess any information about the size of the localization zone and, therefore, an intrinsic material length-scale measure that limits the size of this zone has to be incorporated. Several localization limiters, i.e., as means of preserving the well-posedness and discretization sensitivity in (initial) boundary value problems for strain softening media, that introduce explicit or implicit length-scale measures have been proposed in the literature to accommodate this problem. They include but are not limited to: rate-dependent models (e.g., Perzyna, 1963; Needleman, 1988; Loret and Prevost, 1990; Prevost and Loret, 1990; Sluys, 1992; Wang et al., 1996; Dornowski and Perzyna, 2000; Glema et al., 2000; Wang and Sluys, 2000); integral nonlocal models (e.g., Kroner, 1967; Eringen and Edelen, 1972; Pijaudier-Cabot and Bazant, 1987; Bazant and Pijaudier-Cabot, 1988; Bazant and Ozbolt, 1990; Bazant and Jirasek, 2002; Jirasek and Rolshoven, 2003); and nonlocal gradient-dependent models (e.g., Aifantis, 1984; Lasry and Belytschko, 1988; de Borst and Sluys, 1991; Mühlhaus and Aifantis, 1991; de Borst and Mühlhaus, 1992; Zbib and Aifantis, 1992; de Borst and Pamin, 1996; Kuhl et al., 2000; Lacey et al., 2000; Voyiadjis et al., 2001).

The incorporation of viscosity (rate-dependency) allows the spatial difference operator in the governing equations to retain its ellipticity and the initial value problem (the Cauchy problem) is well-posed. This is because viscosity introduces implicitly a length-scale measure that limits localization in dynamic or quasi-static problems: $\ell = c\eta^{\rm v}$ where c denotes the velocity of the propagation of the elastic waves in the material and η^{v} is the relaxation time for mechanical disturbances, which is directly related to the viscosity of the material (Loret and Prevost, 1990; Prevost and Loret, 1990). Sluys (1992) has also demonstrated that this viscosity length-scale effect can be related to the spatial attenuation of waves that have real wave speeds in the softening regime. Consequently, any rate dependence in the constitutive law combined with inertial effects introduces an implicit length-scale that gives the possibility to obtain mesh-insensitive results (e.g., Needleman, 1988; Loret and Prevost, 1990; Prevost and Loret, 1990; Wang et al., 1996; Dornowski and Perzyna, 2000; Glema et al., 2000; Wang and Sluys, 2000). The rate-independent inelastic response is obtained as a limit case when the relaxation time is equal to zero, i.e., $\eta^{v} = 0$; hence, the theory of viscoinelasticity offers the localization limiter (or regularization procedure) for the solution of dynamic initial boundary value problems. It is imperative, however, to emphasize that rate-dependent theories are neither necessary nor sufficient in taking into account the microscopic interactions with other material points in the vicinity of that point. In other words, viscosity is not necessarily successful in capturing the effect of size and spacing of microdefects on the overall response of the material (nonlocality). The nonlocal theory can thus be used to remedy this situation.

The integral nonlocal theory involves an infinitely extended zone of nonlocal action that may be approximated by the truncated Taylor series expansion, giving rise to the so-called gradient-dependent theory. The gradient approach typically retains in the constitutive equations terms of high-order gradients with coefficients representing length-scale measures of the deformation microstructure. Aifantis (1984) was one of the first to study the gradient regularization in solid mechanics. Other researchers have contributed substantially to the gradient approach with emphasis on numerical aspects of the theory and its implementation in finite element codes: Lasry and Belytschko (1988), Aifantis (1992), Zbib and Aifantis (1992), and de Borst and coworkers (e.g., de Borst and Sluys, 1991; de Borst and Mühlhaus, 1992; de Borst et al., 1993; Pamin, 1994; de Borst and Pamin, 1996; Peerlings et al., 1996; Fleck and Hutchinson, 1997; de Borst et al., 1999). In addition, the recent works of Wang et al. (1998), Aifantis et al. (1999), Bammann et al. (1999), Ganghoffer (1999), Gao et al. (1999), Acharya and Bassani (2000), Askes et al. (2000), Geers et al. (2000), Kuhl et al. (2000), Oka et al. (2000), Svedberg and Runesson (2000), Chen

and Wang (2002), and Di Prisco (2002) should be included here. Gradient thermodynamic models were also introduced by Fremond and Nedjar (1996), Gurtin (2002, 2003), and Voyiadjis and his coworkers (e.g., Voyiadjis et al., 2001, 2003, 2004). Moreover, reference is made to interesting contributions on the physical origin of the length-scale in gradient plasticity theories made by Voyiadjis and Abu Al-Rub (2004) and Abu Al-Rub and Voyiadjis (2004).

Explicit length-scale measures via nonlocal gradient-dependent theory and/or implicit length-scale measures via viscoinelasticity theory can thus be considered either as regularization parameters or localization limiters (computational point of view), or as micromechanical parameters to be determined from observed shear-band widths or size effect experiments (physical point of view).

The objective of this article is to present a micromechanically based constitutive model for the modeling of heterogeneous media that assesses a strong coupling between (visco) plasticity and (visco) damage for high velocity impact related problems while considering the discontinuities on the macroscale level. The essential aspects of interest here can all be examined within the context of: (1) finite deformation kinematics; (2) rapid time variations in temperature, strain, strain rate, and other field variables; (3) equation of state; (4) thermal and damage softening; (5) strong viscoplasticity and viscodamage coupling; (6) long range microstructural interactions through the use of the nonlocal continua; and (7) numerical stability through the use of regularization approaches (i.e., using viscosity and gradient localization limiters). This can be effectively characterized through a thermodynamic framework for the development of a nonlinear continuum hypoelasto-thermo-viscoplastic and thermoviscodamage based failure model. The constitutive equations are derived from the first and second laws of thermodynamics, the expression of the Helmholtz free energy, the Clausius–Duhem inequality, the maximum dissipation principle, the generalized normality rule, and the balance heat equation. All the thermodynamic equations are expressed in the spatial configuration. The evolution laws are implemented in a finite deformation framework based on the additive decomposition of the spatial rate of deformation into elastic, viscoplastic, and viscodamage components. Furthermore, the constitutive equations for the damaged material are written according to the principle of strain energy equivalence between the virgin material and the damaged material. Extension of this concept to nonlocal continua is also discussed. In addition, the nonlocality is introduced here through the viscoplasticity and viscodamage hardening variables. The second-order gradients in the gradient-dependent theory are mainly considered in this study; while the first-order gradients are disregarded since the isotropic nonlocal influence is assumed. The local viscoplasticity and viscodamage hardening variables and their corresponding second-order gradients are considered mathematically dependent on each other, but each gives different physical interpretations that lead to different evolution equations allowing us to computationally introduce independently the influence of the macroscale and mesoscale levels.

The developments in this first part of this work are focused on the consideration of nonlocal plastic-damage modeling in the finite deformation range for rate- and temperature-dependent materials. Presented in Part II are the computational aspects and numerical algorithms for the integration of the resulting constitutive equations with applications to impact related problems.

The next section introduces the nonlocal concepts, extension of the non-local concept to anisotropic damage, and a completely consistent thermodynamic framework for the hypoelasto-viscoplastic and viscodamage material behavior with rate, thermal, and pressure effects for impact related problems using the nonlocal gradient-dependent theory. The rate-type of stress–strain constitutive relation is derived, the heat balance equation is formulated and a failure criterion is proposed. All these are presented in the subsequent sections. Conclusions are also provided.

NONLOCAL CONSTITUTIVE MODELING FOR DYNAMIC LOADING

Weak Nonlocal Formulation using the Gradient Approach

Materials with a microstructure are nonlocal in behavior due to the interplay of characteristic lengths including sizes or spacing of defect clusters, grain sizes, fiber spacing, etc. As traditional continuum mechanics does not contain characteristic lengths, the use of the nonlocal concept is required to introduce a microstructure characteristic length and to introduce long-range microstructural interactions where the stress response at a material point is assumed to depend on the state of its neighborhood in addition to the state of the material point itself. In this article, the use of the nonlocal continuum theory is made. Integral-type nonlocal models replace one or more variables (typically, state variables) by their nonlocal counterparts obtained by weighted averaging over a spatial neighborhood of each point under consideration. If A(x) is some 'local' field in a domain V, the corresponding nonlocal field, $\widehat{A}(x)$, is defined as follows:

$$\widehat{A}(x) = \frac{1}{V} \int_{V} \mathbf{h}(\xi) A(x + \xi) \, \mathrm{d}V \quad \text{with} \quad V(\xi) = \int_{V} \mathbf{h}(\|\xi\|) \, \mathrm{d}V \tag{1}$$

The superimposed hat denotes the spatial nonlocal operator, and $h(\xi)$ is a nonlocal weight function that decays smoothly with distance $\|\xi\|$. In Equation (1) ξ is the vector pointing to the infinitesimal volume dV. The weight function is often taken as the Gaussian error distribution function

$$h(\|\xi\|) = \exp\left(\frac{-n_{\dim}\|\xi\|^2}{2\ell^2}\right) \tag{2}$$

where ℓ is called the internal length of the nonlocal continuum, which sets the averaging volume or the size of inhomogeneity, and $n_{\rm dim}$ is the spatial dimension of the problem (1, 2, or 3). Theoretically, the Gauss function in Equation (2) has an unbound support, i.e., its interaction length is $\zeta \to \infty$. In practical calculations, the weight function is truncated at the distance where its value becomes negligible.

Gradient formulations are found when the local field $A(x + \xi)$ in Equation (1) is expanded in a Taylor series around x, such that:

$$A(x + \xi) = A(x) + \nabla A(x)\xi + \frac{1}{2!}\nabla^{2}A(x)\xi\xi + \frac{1}{3!}\nabla\nabla^{2}A(x)\xi\xi\xi + \frac{1}{4!}\nabla^{2}\nabla^{2}A(x)\xi\xi\xi\xi \dots$$
(3)

where ∇ is the first-order gradient operator and ∇^2 denotes the second-order gradient (Laplacian) operator. The above Taylor series expansion of the local variable A is then substituted in the nonlocal spatial averaging, Equation (1). Since an infinite isotropic body is considered here, when conducting the integration of Equation (1) with infinite integration intervals, all of the odd terms in Equation (3) (i.e., the second and fourth terms on the right-hand side of Equation (3)) vanish. Consequently, \hat{A} reduces to:

$$\widehat{A} = \frac{1}{V} \int_{V} \mathbf{h}(\xi) A(x) \, \mathrm{d}V + \frac{1}{2!V} \int_{V} \mathbf{h}(\xi) \nabla^{2} A(x) \xi \xi \, \mathrm{d}V \tag{4}$$

where the terms of fourth- and higher-order have been neglected.

Substituting Equation (2) into Equation (4) and integrating from $-\infty$ to ∞ leads to

$$\widehat{A} = A + \frac{1}{2}\ell^2 \nabla^2 A \tag{5}$$

where ℓ is the internal material length-scale, which weights each component of the gradient term identically. The role of the material length-scale in

solving the impact damage problem and in preserving the objectivity of the continuum modeling and numerical simulation of the localization problem is the main concern of this article.

If a more general tensorial character for the nonlocal weight function not necessarily confined to the expressions in Equations (2) is assumed, a different weighting of the individual coefficients is obtained. In other words, replacing the traditional averaging operator in Equation (1) by a more complicated implicit scheme, which takes into account not only the distance $\|\xi\|$, but also the relative orientation of the principal strain axes at x is suggested. This modification can lead to an improved performance, especially when anisotropic influence needs to be simulated. In this work, attention to standard nonlocal averaging of Equation (1) is restricted.

An attempt is made here to account for the effect of non-uniform distribution of microdefects on the overall macroscale response by assuming the thermoelastic Helmholtz free-energy density, Ψ , to depend not only on the macroscopic response associated with the internal state variable A, but also on its macroscopic spatial second-order gradient (or Laplacian) $\nabla^2 A$. This will be detailed in the subsequent sections of this article.

Nonlocal Effective Configuration

Continuum damage models based on the effective stress space (undamaged configuration) were introduced by Kachanov (1958) and later by Rabotnov (1968) who were the first to introduce for the isotropic case a one-dimensional variable, ϕ , which may be interpreted as the effective surface density of microdamage per unit volume (Voyiadjis and Venson, 1995), such that the effective Kirchhoff stress tensor, $\bar{\tau}$, is expressed as follows:

$$\bar{\tau}_{ij} = \frac{\tau_{ij}}{1 - \phi} \tag{6}$$

However, Equation (6) is a mathematical definition of the effective stress although it may be interpreted as the uniform (average) stress acting on an effective area of the material (Abu Al-Rub and Voyiadjis, 2003). To give it a general physical meaning, it is necessary to use the corresponding damage-free material (i.e., virgin material) in the mesoscale to represent the 'effective' concept of Equation (6) for a macroscopically damaged material. Thus, a proper correlating hypothesis between two material scale levels can be obtained using the nonlocal damage variable $\hat{\phi}$. It is then important to emphasize that Kachanov's definition given by Equation (6) can be

generalized to a nonlocal one, for the case of isotropic damage and under a general state of stress, as follows:

$$\bar{\tau}_{ij} = \frac{\tau_{ij}}{1 - \hat{\phi}} \tag{7}$$

where the possible approaches in interpreting the nonlocal quantity $\hat{\phi}$ will be discussed thoroughly later in this article. However, it was shown by Ju (1989) that two independent damage parameters are needed to describe this case adequately for local continuum.

To ensure a more general formulation of the principles of damage mechanics, the case of anisotropic damage will be assumed in this work (Chow and Wang, 1987; Voyiadjis and Kattan, 1992a, b). Therefore, the anisotropic phenomenon of the microdamage (i.e., microcracks and microvoids) distribution in the material is interpreted using a nonlocal symmetric second-order damage tensor, $\hat{\phi}$.

The linear elastic constitutive equations for the damaged material are expressed by Equation (6). That is, the damaged material is modeled using the constitutive laws of the effective undamaged material in which the Kirchhoff stress tensor, τ , can be replaced by the effective stress tensor, $\bar{\tau}$ (Murakami and Ohno, 1981) as follows:

$$\bar{\tau}_{ij} = \hat{M}_{ikjl} \, \tau_{kl} \tag{8}$$

where \widehat{M} is the nonlocal fourth-order damage-effect tensor. The tensor \widehat{M} , which is then expressed in terms of $\widehat{\phi}$, characterizes the notion of non-uniform distribution and interaction of microcracks and microvoids over multiple length-scales at which first and second nearest neighbor effects of nonlocal character are significant, similar to the homogenization theory.

Many different expressions for the local M have been proposed in the literature in order to symmetrize the effective stress tensor, $\bar{\tau}$. A comprehensive review of the most widely used expressions are presented by Voyiadjis and Park (1997). The following expression for M is adopted here for M due to its attractiveness in the mathematical formulation (Abu Al-Rub and Voyiadjis, 2003), such that:

$$\hat{M}_{ikjl} = 2 \left[\left(\delta_{ik} - \hat{\phi}_{ik} \right) \delta_{jl} + \delta_{ik} \left(\delta_{jl} - \hat{\phi}_{jl} \right) \right]^{-1} \tag{9}$$

where $\hat{\phi}$ is the nonlocal damage variable whose evolution will be defined later. Note that the fourth-order tensor \hat{M} exhibits the major symmetries only (i.e., $\hat{M}_{ikjl} = \hat{M}_{jlik}$).

For finite strain problems and assuming small elastic strains (usually accepted for metals and other materials subjected to high strain-rate loading), the additive decomposition of the total rate of deformation tensor, d, into elastic part, d^e , and viscoinelastic part, d^{vi} is assumed, such that:

$$d_{ij} = d_{ij}^{\mathrm{e}} + d_{ij}^{\mathrm{vi}} \tag{10}$$

The elastic rate of deformation, d^e , is the reversible part attributed to elastic distortions, microcracks closure, and microvoids contraction upon unloading (but not healing). On the other hand, the viscoinelastic rate of deformation, d^{vi} , designates the irreversible part of the total strain attributed to viscoplastic distortions and viscodamage strains and is characterized by the lack of microcrack closure and microvoid contraction which cause permanent deformations. The lack of microcrack closure and microvoid contraction can be due to the constraints set up by the interacting microcracks, microvoids, dislocation movements, and external/internal interfaces (Abu Al-Rub and Voyiadjis, 2003). Therefore, the viscoinelastic part of deformation can be further decomposed as follows:

$$d_{ij}^{\text{vi}} = d_{ij}^{\text{vp}} + d_{ij}^{\text{vd}} \tag{11}$$

where d^{vp} is the viscoplastic rate of deformation and d^{vd} is the viscodamage rate of deformation. Analogous to the additive decomposition in Equations (10) and (11), the spatial total strain tensor, e, can be also decomposed as follows:

$$e_{ij}^{e} = e_{ij}^{e} + e_{ij}^{vi} = e_{ij}^{e} + e_{ij}^{vp} + e_{ij}^{vd}$$
 (12)

To derive the transformation relations between the damaged and the hypothetical undamaged (effective) states of the material, the elastic energy equivalence hypothesis (Sidoroff, 1980) is utilized here. This hypothesis assumes that each of the elastic energy density in terms of effective and nominal stress and corresponding strain quantities must be equal, such that we express the effective elastic strain tensor, \bar{e}^e , in terms of the elastic strain tensor, e^e , as follows:

$$\bar{e}_{ij}^{\mathrm{e}} = \hat{M}_{ikjl}^{-1} e_{kl}^{\mathrm{e}} \tag{13}$$

By using the elastic strain energy equivalence principle (Sidoroff, 1980), we can write the fourth-order tensor of the elastic-damage modulus, \mathbb{C} , as follows:

$$\mathbb{C}_{ijkl} = \hat{M}_{imin}^{-1} \bar{\mathbb{C}}_{mnpq} \hat{M}_{pkql}^{-1} \tag{14}$$

where

$$\widehat{M}_{ikjl}^{-1} = \frac{1}{2} \left[\left(\delta_{ik} - \widehat{\phi}_{ik} \right) \delta_{jl} + \delta_{ik} \left(\delta_{jl} - \widehat{\phi}_{jl} \right) \right]$$
 (15)

and $\bar{\mathbb{C}}$ is the undamaged fourth-order elastic modulus tensor. It is noteworthy that the elastic-damage stiffness, \mathbb{C} , exhibits the major and minor symmetries similar to the elastic stiffness, $\bar{\mathbb{C}}$.

Viscoplasticity and Damage Internal State Variables

In this work, thermal, elastic, viscoplastic (rate-dependent plasticity), and viscodamage (rate-dependent damage or creep damage) material behavior is considered. This means that the stress path, strain rate, temperature, pressure material dependence, and nonlinear material response are all considered. Thus, the dependent constitutive variables are functions of the elastic strain tensor, e^e , the absolute temperature, T, the temperature gradient vector, ∇T , the measure of volumetric deformation, $J = \det(F)$ with F is the deformation gradient, and n_{int} – of phenomenological nonlocal internal state variables, $\hat{\aleph}_k$ ($k = 1, \ldots, n_{\text{int}}; n_{\text{int}} \geq 1$). Hence, within the thermodynamic framework and considering the assumption of infinitesimal elastic strains, the Helmholtz free-energy density function can be written as:

$$\Psi = \tilde{\Psi} \Big(e_{ij}^{e}, T, \nabla_{i} T, J; \hat{\aleph}_{k} \Big)$$
 (16)

Since the main objective is to provide an adequate (i.e., physical) characterization of material defects (microcracks, microvoids, mobile and immobile dislocation densities) in terms of size, orientation, distribution, spacing, interaction among defects, and so forth, a finite set of nonlocal internal state variables, $\hat{\aleph}_k$, representing either a scalar or a tensorial variable are assumed. These variables should include the nonlocal effect through the proposed gradient-dependent approach presented in the previous sections. Therefore, motivated by the derived nonlocal equation, Equation (5), it is assumed that $\hat{\aleph}_k$ is also decomposed into a local part, Ξ_n , and a Laplacian part, $\nabla^2\Xi_n$, such that:

$$\widehat{\aleph}_k = \widetilde{\aleph}_k \big(\Xi_n, \nabla^2 \Xi_n\big) \tag{17}$$

where Ξ_n is a set of viscoplasticity and viscodamage hardening/softening internal state variables, and $\nabla^2 \Xi_n$ is the corresponding second-order gradient (Laplacian) of Ξ_n . The state variables in this gradient-enhanced approach are no longer independent; therefore, special care must be taken to

properly account for state variable coupling between Ξ_n and $\nabla^2 \Xi_n$ (Lacey et al., 2000). Moreover, setting Ξ_n and $\nabla^2 \Xi_n$ as dependent internal state variables allows us to computationally introduce the effects of the material defects in the mesoscale on the macroscale response, which gives different physical interpretations that guides us to different evolution equations for Ξ_n and $\nabla^2 \Xi_n$. This postulate is motivated through the fact that certain internal state variables such as the statistically stored dislocation (SSD) and geometrically necessary dislocation (GND) densities do not necessarily have the same evolution equations, but they are dependent on each other (Abu Al-Rub and Voyiadjis, 2004; Voyiadjis and Abu Al-Rub, 2004).

The sets of macro internal state variables, Ξ_n and $\nabla^2 \Xi_n$, are postulated, respectively as:

$$\Xi_n = \tilde{\Xi}_n(p, \alpha_{ij}, r, \Gamma_{ij}, \phi_{ij})$$
(18)

$$\nabla^2 \Xi_n = \nabla^2 \tilde{\Xi}_n (\nabla^2 p, \nabla^2 \alpha_{ij}, \nabla^2 r, \nabla^2 \Gamma_{ij}, \nabla^2 \phi_{ij})$$
 (19)

where p denotes the accumulative viscoplastic strain and α denotes the flux of residual stress (backstress). The scalar p is associated with isotropic hardening/softening (size of the yield surface) and α with kinematic hardening (translation of the yield surface) in the viscoplastic flow process. Similarly, r denotes the accumulative viscodamage and Γ denotes the flux of residual stress (damage kinematic hardening) in the viscodamage growth process. The second-order gradients, $\nabla^2 \Xi_n$, are suitable for the description of the strain-softening regime. The assumed dependence of the Helmholtz free energy on the distinct variables $\nabla^2 \Xi_n$ is also motivated by the necessity to include length-scale measures into the equations of state that link the mesoscale interactions to the macroscale viscoplasticity and viscodamage, which cannot be captured by Ξ_n variables alone.

One of the current main challenges in constitutive modeling is the determination of the evolution equations for the assumed state variables that appeared in the Helmholtz free-energy density function (Equations (16)–(19)). This can be effectively achieved, so far, through the thermodynamic principles (Coleman and Gurtin, 1967; Lemaitre and Chaboche, 1990; Lubliner, 1990; Simo and Hughes, 1998; Belytschko et al., 2000; Doghri, 2000). The Clausius–Duhem inequality can be written in the finite deformation context as:

$$\sigma_{ij}d_{ij} - \rho(\dot{\Psi} + \eta \dot{T}) - \frac{1}{T}q_i\nabla_i T \ge 0$$
 (20)

where ρ , η , and \boldsymbol{q} are the mass density, the specific entropy, and the heat flux vector, respectively.

For the purpose of describing the viscoinelastic behavior of the materials involved in dynamic loading, an additive decomposition of specific free-energy function, Ψ , into thermoelastic, thermoviscoplastic, and thermoviscodamage parts is assumed here (e.g., Voyiadjis and Kattan, 1992a, b, 1999; Hansen and Schreyer, 1994; Voyiadjis and Park, 1999; Abu Al-Rub and Voyiadjis, 2003), such that:

$$\widetilde{\Psi}\left(e_{ij}^{e}, T, \nabla_{i}T, J; \widehat{\aleph}_{k}\right) = \widetilde{\Psi}^{te}\left(e_{ij}^{e}, J^{e}, T, \nabla_{i}T, \phi_{ij}, \nabla^{2}\phi_{ij}\right)
+ \widetilde{\Psi}^{tvp}\left(T, \nabla_{i}T, p, \nabla^{2}p, \alpha_{ij}, \nabla^{2}\alpha_{ij}, \phi_{ij}, \nabla^{2}\phi_{ij}\right)
+ \widetilde{\Psi}^{tvd}\left(T, \nabla_{i}T, r, \nabla^{2}r, \Gamma_{ij}, \nabla^{2}\Gamma_{ij}, \phi_{ij}, \nabla^{2}\phi_{ij}\right)$$
(21)

where Ψ^{te} is the thermoelastic stored energy which is assumed to equal the thermoelastic stored energy in the undamaged configuration, while Ψ^{tvp} and Ψ^{tvd} are energies stored due to material hardening in viscoplasticity and viscodamage deformation mechanisms, respectively.

Assuming incompressible inelastic deformation (det $F^{vi} = 1$), $\Psi(e^e_{ij}, T, \nabla_i T, J; \hat{\aleph}_k) = \tilde{\Psi}(e^e_{ij}, T, \nabla_i T, J^e; \hat{\aleph}_k)$ could be written. Furthermore, it should be noted that Equation (21) is a partially decoupled form of the specific free energy Ψ . There is no state coupling between viscoplasticity and elasticity, but the state coupling of viscodamage with the elastic and viscoplastic stored energies strongly appears in the above decomposition. In particular, the damage variables ϕ and $\nabla^2 \phi$ appear in all portions of Ψ and the other internal state variables are expressed in the current, deformed, and damaged configurations. The variables ϕ and $\nabla^2 \phi$ appear implicitly in Ψ^{tvp} through the evolution of its set of internal state variables as will be shown in a later section.

General Thermodynamic Formulation

According to the definition given in the previous section for Ψ , the time derivative of Equation (16) with respect to its internal state variables is given by:

$$\dot{\Psi} = \frac{\partial \Psi}{\partial e_{ij}^{e}} \dot{e}_{ij}^{e} + \frac{\partial \Psi}{\partial J^{e}} \dot{J}^{e} + \frac{\partial \Psi}{\partial T} \dot{T} + \frac{\partial \Psi}{\partial \nabla_{i} T} \nabla_{i} \dot{T} + \frac{\partial \Psi}{\partial \aleph_{k}} \dot{\widehat{\aleph}}_{k}$$
(22)

However, the invariance of $\dot{\Psi}$ requires objective derivatives for the tensors. To avoid excessive contribution to the dissipated energy, rotational derivatives are used here, such that:

$$\dot{\Psi} = \frac{\partial \Psi}{\partial e_{ij}^{e}} \dot{e}_{ij}^{e} + \frac{\partial \Psi}{\partial J^{e}} \dot{J}^{e} + \frac{\partial \Psi}{\partial T} \dot{T} + \frac{\partial \Psi}{\partial \nabla_{i} T} \nabla_{i}^{\nabla} T + \frac{\partial \Psi}{\partial \hat{\aleph}_{k}} \hat{\aleph}_{k}^{\nabla}$$
(23)

where $(^{\nabla})$ designates the corotational derivative, which is objective under any rotation. Note that in Equation (23), the corotational derivative of the spatial elastic strain tensor, $\stackrel{.}{e}$, defines the elastic rate of deformation tensor, $\stackrel{.}{d}^e$. Substituting the rate of the Helmholtz free-energy density, Equation (22), into the Clausius–Duhem inequality, Equation (20), along with Equation (10) and $\stackrel{.}{J}^e = J^e d^e_{ij} \delta_{ij}$, the following thermodynamic constraint is obtained:

$$\left(\sigma_{ij} - \rho \frac{\partial \Psi}{\partial e_{ij}^{e}}\right) d_{ij}^{e} + \sigma_{ij} d_{ij}^{vi} - \rho \frac{\partial \Psi}{\partial J^{e}} J^{e} d_{kk}^{e} - \rho \left(\frac{\partial \Psi}{\partial T} + \eta\right) \dot{T}
- \rho \frac{\partial \Psi}{\partial \nabla_{i} T} \nabla_{i}^{\nabla} T - \rho \frac{\partial \Psi}{\partial \aleph_{k}} \hat{\aleph}_{k}^{v} - \frac{q_{i}}{T} \nabla T \ge 0$$
(24)

Multiplying both sides of Equation (24) by the Jacobian determinant of F (i.e., $J = \rho_{\rm o}/\rho$) and assuming that the axiom of entropy production holds, then the above inequality equation results in the following thermodynamic state laws:

$$\sigma_{ij} = \rho \frac{\partial \Psi}{\partial e_{ij}^{e}} \quad \text{or} \quad \tau_{ij} = J \sigma_{ij} = \rho_{o} \frac{\partial \Psi}{\partial e_{ij}^{e}}$$
 (25)

$$P = -\rho_0 \frac{\partial \Psi}{\partial J^e}; \quad \eta = -\frac{\partial \Psi}{\partial T}; \quad \frac{q_i}{\dot{T}} = \rho_0 \frac{\partial \Psi}{\partial \nabla_i T}; \quad \sum_k = \rho_0 \frac{\partial \Psi}{\partial \hat{\aleph}_k}$$

$$(k = 1, \dots, 10) \tag{26}$$

The above equations describe the relations between the state variables and their associated thermodynamic conjugate forces. The Cauchy stress tensor, σ , or the Kirchhoff stress tensor, τ , are measures of the elastic changes in the internal structure; P is the thermodynamic pressure conjugate to the elastic change in volume due to high energy impacts. The state laws of the assumed internal state variables, Equation (26)₄, are expressed in Table 1 in terms of their associated internal state variables. The superscript 'g' in Table 1 indicates the thermodynamic conjugate force corresponding to the second-order gradient or Laplacian of the assumed internal state variables. The conjugate forces R, R^g , X, and X^g are measures of viscoplastic changes in the internal structure, while K, K^g , H, and H^g are measures of the viscodamage changes in the internal structure. Y and Y^g are the damage forces, known as the energy release rates resulting from the elastic-damage changes in the internal structure.

Table 1. Thermodynamic state laws of viscoplasticity and viscodamage.

| Plasticity Isotropic hardening | $R= ho_{ m o}rac{\partial\Psi^{ m tvp}}{\partial m p}$ | $R^{ m g}= ho_{ m o}rac{\partial\Psi^{ m tvp}}{\partial abla^2p}$ |
|--------------------------------|---|---|
| Kinematic hardening | $X_{ij} = \rho_0 \frac{\partial \dot{\Psi}^{\text{tvp}}}{\partial \alpha_{ij}}$ | $X_{ij}^{g} = \rho_{o} \frac{\partial \Psi^{tvp}}{\partial \nabla^2 \alpha_{ij}}$ |
| Damage Isotropic hardening | $\mathcal{K} = ho_{o} rac{\partial \Psi^{tvd}}{\partial r}$ | $K^{\mathrm{g}} = ho_{\mathrm{o}} rac{\partial \Psi^{\mathrm{tvd}}}{\partial \nabla^{2} r}$ |
| Kinematic hardening | $H_{ij} = ho_0 \frac{\partial \Psi^{\text{tvd}}}{\partial \Gamma_{ij}}$ | $H_{ij}^{g} = \rho_{o} \frac{\partial \Psi^{tvd}}{\partial \nabla^{2} \Gamma_{ij}}$ |
| Damage force | $-Y_{ij}= ho_{\mathbf{o}}rac{\partial\Psi^{\mathrm{te}}}{\partial\phi_{ij}}$ | $-Y_{ij}^{g} = \rho_{o} \frac{\partial \Psi^{te}}{\partial \nabla^{2} \phi_{ij}}$ |

Gibbs relation and the Clausius-Duhem inequality are finally written, respectively, as follows:

$$\rho_{o}\dot{\Psi} = \tau_{ij}\left(d_{ij} - d_{ij}^{vi}\right) + PJ^{e}d_{kk}^{e} - \rho_{o}\eta\dot{T} + \frac{q_{i}}{\dot{T}}\nabla_{i}^{\nabla}T + \Pi_{int}$$
 (27)

$$\Pi = \tau_{ij}d_{ij}^{\text{vi}} + PJ^{\text{e}}d_{kk}^{\text{e}} - \Pi_{\text{int}} - q_i \left(\frac{\nabla_i T}{T} + \frac{\nabla_i^{\text{v}} T}{\dot{T}}\right) \ge 0$$
 (28)

where Π is the total dissipation energy and $\Pi_{\text{int}} = \sum_{k=1}^{10} \Sigma_k \, \aleph_k$ is the internal viscoinelastic dissipation energy. To this end, the following split is proposed: $n_{\text{int}} = n_{\text{int}}^{\text{vp}} + n_{\text{int}}^{\text{vd}}$, where $n_{\text{int}}^{\text{vp}}$ and $n_{\text{int}}^{\text{vd}}$ refer to the number of internal state variables related to viscoplastic and viscodamage effects, respectively. In this context, this assumption leads to rewriting the dissipation energy, Π , as the summation of dissipations due to mechanical (viscoplasticity and viscodamage) and thermal (heat conduction) effects as:

$$\Pi = \Pi^{vp} + \Pi^{vd} + \Pi^{th} \ge 0, \tag{29}$$

where

$$\Pi^{\text{vp}} = \tau_{ij} d_{ij}^{\text{vp}} + P J^{e} d_{kk}^{e} - R \dot{p} - R^{g} \nabla^{\nabla} p - X_{ij} \alpha_{ij}^{\nabla} - X_{ij}^{g} \nabla^{\nabla} \alpha_{ij} \ge 0,$$
 (30)

$$\Pi^{\text{vd}} = \tau_{ij} d_{ij}^{\text{vd}} + Y_{ij} \phi_{ij}^{\text{v}} + Y_{ij}^{\text{g}} \nabla^{\nabla} \phi_{ij} - K \dot{r} - K^{\text{g}} \nabla^{\nabla} r - H_{ij} \Gamma_{ij}^{\nabla} - H_{ij}^{\text{g}} \nabla^{\nabla} \Gamma_{ij}^{\nabla} \geq 0, \quad (31)$$

$$\Pi^{\text{th}} = -q_i \left(\frac{\nabla_i T}{T} + \frac{\nabla^{\nabla}_i T}{\dot{T}} \right) \ge 0.$$
 (32)

This result requires all viscoinelastic work to dissipate away as heat, except for that energy which is stored because of the rearrangement of the material internal structure. Although, we write the thermoviscoinelastic dissipation function, Π, in the decoupled form as shown by Equation (29), this does not imply that the corresponding physical mechanisms are decoupled. Strong coupling does occur in the viscoplastic potential given by Equation (30) between viscoplasticity and viscodamage since the conjugate forces and their associated state variables are expressed in the current, deformed, and damaged configuration of the material. Two additive damage mechanisms, hence, are introduced in the dissipation function, Equation (29); one mechanism is coupled with viscoplasticity and the other occurs independent of viscoplastic deformation.

It is clearly seen that the definition of Ψ and consequently the evolution of $\hat{\aleph}_k$ $(k=1,\ldots,10)$ are essential features of the formulation to describe the thermomechanical/microstructural behavior of the material involved in the deformation process. The associative evolution laws of $\boldsymbol{d}^{\text{vi}}$ and $\boldsymbol{\phi}$ can be obtained by utilizing the calculus of several variables with Lagrange multipliers $\hat{\lambda}^{\text{vp}}$ and $\hat{\lambda}^{\text{vd}}$. The inelastic dissipation function $\Pi^{\text{I}} = \Pi^{\text{vp}} + \Pi^{\text{vd}}$ (Equation (29)) is subjected to two constraints, namely f=0 and g=0 (e.g., Voyiadjis and Kattan, 1992a, b):

$$\Omega = \Pi^{\text{vp}} + \Pi^{\text{vd}} - \dot{\lambda}^{\text{vp}} f - \dot{\lambda}^{\text{vd}} g \tag{33}$$

We now make use of the maximum viscoinelastic dissipation principle (e.g., Simo and Honein, 1990; Simo and Hughes, 1998), which states that the actual state of the thermodynamic forces (τ, Y) is that which maximizes the inelastic dissipation function over all other possible admissible states. We maximize, therefore, the objective function Ω by using the necessary conditions as follows:

$$\frac{\partial \Omega}{\partial \tau_{ij}} = 0$$
 and $\frac{\partial \Omega}{\partial Y_{ij}} = 0$ (34)

Substitution of Equation (33) into Equation (34) along with Equations (30) and (31) yields the thermodynamic laws corresponding to the evolution of the viscoinelastic rate of deformation $(\mathbf{d}^{\text{vi}} = \mathbf{d}^{\text{vp}} + \mathbf{d}^{\text{vd}})$ and the viscodamage variable ϕ . Equation (34)₁ gives the viscoinelastic strain rate as follows:

$$d_{ij}^{\text{vp}} = \dot{\lambda}^{\text{vp}} \frac{\partial f}{\partial \tau_{ij}}, \qquad d_{ij}^{\text{vd}} = \dot{\lambda}^{\text{vd}} \frac{\partial g}{\partial \tau_{ij}}$$
 (35)

Similarly, Equation (34)₂ gives the viscodamage evolution law as follows:

where

$${}^{(1)} \phi_{ij} = \dot{\lambda}^{\text{vp}} \frac{\partial f}{\partial Y_{ij}}, \qquad {}^{(2)} \phi_{ij} = \dot{\lambda}^{\text{vd}} \frac{\partial g}{\partial Y_{ij}}$$

$$(37)$$

The functions f and g are the dynamic viscoplastic and viscodamage loading surfaces that will be defined in later sections, respectively.

As a result we define, respectively, the conventional equivalent viscoplastic strain rate, \dot{p} , and the accumulative viscodamage rate, \dot{r} , as follows (Voyiadjis and Deliktas, 2000):

$$\dot{p} = \sqrt{\frac{2}{3}} d_{ij}^{\text{vi}} d_{ij}^{\text{vi}}, \qquad \dot{r} = \sqrt{\phi_{ij} \phi_{ij}}$$
(38)

Next, to obtain non-associative rules for viscoplasticity and viscodamage local hardening variables (p, α, r, Γ) , which give a more realistic characterization of the material response in the deformation process, we assume the existence of a viscoplastic potential F and a viscodamage potential G such that they are, respectively, not equal to f and g. The complementary laws for the evolution of the local internal state variables $(\Xi_n, n=1,\ldots,5)$, summarized in Table 3, are obtained directly from the generalized normality rules. On the other hand, by adopting the assumption of isotropic influence, the complementary laws for the evolution of the second-order gradients of the assumed local internal state variables $(\nabla^2 \Xi_n, n = 1, ..., 5)$ can be directly obtained by operating on the local equations of Table 3 with the Laplacian. Similarly, ∇^2_{ab} can be obtained from Equation (37). The resulting evolution laws are listed in Table 3. By doing this, we enhance the coupling between the evolutions of Ξ_n and $\nabla^2 \Xi_n$, which will be thoroughly demonstrated in the subsequent sections and the second part of this work.

Specific Free-energy Function

We consider now a generic hypoelasto-thermo-viscoplastic and thermo-viscodamage model based on the general thermodynamic framework developed in the previous sections.

As it is clearly seen from the previous section, the complexity of a model is directly determined by the form of the Helmholtz free energy Ψ and by the number of conjugate pairs of variables. Therefore, the definition of Ψ constitutes a crucial point of the formulation since it is the basis for the derivation of all constitutive equations to be described in what follows. It is possible to decouple the Helmholtz free energy into a potential function for each of the internal state variable in such a way that an analytical expression for the thermodynamic potential is given as a quadratic form of its internal state variables. However, coupling is possible in the viscoplastic potential or the viscodamage potential if they depend on more than one variable, which makes the evolution equations more complex. Moreover, Chaboche (1991) indicated that an energy Ψ with non-quadratic kinematic hardening variables leads to abnormal results; however, coupling with temperature is not discussed there. As a matter of fact, under high strain rate loading a significant temperature rise is produced due to adiabatic heating, which should be considered in constitutive modeling. Experimental results also indicate that plastic deformation is not the dominating source of heat generation during dynamic deformation, but thermodamage coupling must be considered in the simulation for more accurate comparisons with experiments (Bjerke et al., 2002). In the following, a multiplicative temperature coupling term is introduced in the viscoplasticity and viscodamage hardening state variables for more realistic description of their evolution. The thermoelastic energy, Ψ^{te} , can then be postulated as follows:

$$\rho_{o}\Psi^{te} = \frac{1}{2}e_{ij}^{e}\mathbb{C}_{ijkl}\left(\hat{\boldsymbol{\phi}}\right)e_{kl}^{e} - \beta_{ij}\left(\hat{\boldsymbol{\phi}}\right)e_{ij}^{e}(T - T_{r}) - \eta_{r}(T - T_{r}) - \frac{\rho_{o}}{2T_{r}}c_{p}(T - T_{r})^{2}$$
$$-\frac{1}{2\dot{T}}k_{ij}\nabla_{i}T\nabla_{j}T + c_{v}\left(T^{ig} - T_{r}\right)$$
(39)

On the other hand, the thermoviscoplastic and thermoviscodamage energies, Ψ^{tvp} and Ψ^{tvd} , are assumed, respectively, as follows:

$$\rho_{\rm o}\Psi^{\rm tvp} = \frac{1}{2}a_1p^2\vartheta + \frac{1}{2}b_1(\nabla^2p)^2\vartheta + \frac{1}{2}a_2\alpha_{ij}\alpha_{ij}\vartheta + \frac{1}{2}b_2\nabla^2\alpha_{ij}\nabla^2\alpha_{ij}\vartheta \qquad (40)$$

$$\rho_{o}\Psi^{\text{tvd}} = \frac{1}{2}a_{3}r^{2}\vartheta + \frac{1}{2}b_{3}(\nabla^{2}r)^{2}\vartheta + \frac{1}{2}a_{4}\Gamma_{ij}\Gamma_{ij}\vartheta + \frac{1}{2}b_{4}\nabla^{2}\Gamma_{ij}\nabla^{2}\Gamma_{ij}\vartheta$$
(41)

where $\mathbb{C}(\hat{\phi})$ is the fourth-order damage elastic tensor as a function of $\hat{\phi}$, Equation (14); $\beta(\hat{\phi})$ is the second-order tensor of the thermomechanical coefficients (or sometimes referred to as the tangent conjugate of thermal dilatation) as a function of $\hat{\phi}$; c_p is the specific heat at constant pressure;

 $\eta_{\rm r}$ is the reference entropy; a_k and b_k $(k=1,\ldots,4)$ are the material-dependent constants, which are considered independent of temperature; $T_{\rm r}$ is the reference temperature; $k_{ij}\!=\!k\delta_{ij}$ is the heat conductivity second-rank tensor (k being the conductivity coefficient); ϑ is the homologous temperature defined as $\vartheta=1-(T/T_{\rm m})^n$, where $T_{\rm m}$ is the melting temperature and n is the temperature softening component, which might be assumed different for each hardening mechanism; $c_{\rm v}$ is the specific heat at constant volume; and $T^{\rm ig}$ is chosen to have the form of ideal gas temperature, which can be expressed as follows:

$$T^{ig} = T_{r} \exp\left[\frac{\eta - \eta_{r}}{c_{v}}\right] \left[1 + \varepsilon^{e}\right]^{(\gamma - 1)} \exp\left[(\gamma - 1)\left(\frac{1}{(1 + \varepsilon^{e}) - 1}\right)\right]$$
(42)

In the above equation, $\gamma = c_{\rm p}/c_{\rm v}$ is the ratio of specific heat, where $c_{\rm p}$ is the specific heat at constant pressure. Both $c_{\rm v}$ and $c_{\rm p}$ are related to the gas constant \Re by $\Re = c_{\rm p} - c_{\rm v}$. The above expression is postulated to derive an expression for the equation of state, which relates pressure to specific density. In Equation (42) $\varepsilon^{\rm e} = 1/J^{\rm e} - 1$ is the nominal volumetric elastic strain.

The constitutive equations for the thermoelastic Kirchhoff stress tensor, Equation (25)₂, can be expressed from the thermodynamic potential, Equation (39), as follows:

$$\tau_{ij} = \mathbb{C}_{ijkl} \left(e_{kl} - e_{kl}^{\text{vp}} - e_{kl}^{\text{vd}} \right) - \beta_{ij} (T - T_{\text{r}})$$

$$\tag{43}$$

Furthermore, by using Equations (8), (13), and (14) the stress relation Equation (43) can be written in the effective (undamaged) configuration as follows:

$$\bar{\tau}_{ii} = \bar{\mathbb{C}}_{iikl}\bar{e}_{kl}^e - \bar{\beta}_{ii}(T - T_{\rm r}) \tag{44}$$

where $\bar{\beta} = \hat{M} : \beta$ and $\bar{\beta} = 3K^e\alpha_t \mathbf{1}$ with K^e is the effective bulk modulus, α_t is the coefficient of thermal expansion, and $\mathbf{1}$ is the second-order unit tensor.

Using Equation $(26)_1$ the thermodynamic pressure stress P is given as follows:

$$P = (1 - \gamma)c_{\rm v}T^{\rm ig}\varepsilon^{\rm e} \tag{45}$$

which gives the equation of state necessary for high-impact loading. The equation of state accounts for compressibility effects (changes in density).

The constitutive equation for the heat flux vector \mathbf{q} can be obtained from Equation (26)₃ as follows:

$$q_i = -k_{ij}\nabla_i T \tag{46}$$

which is the well-known Fourier heat conduction law. The negative sign indicates that the heat flow is opposite to the direction of temperature increase.

The state laws of the assumed internal state variables, Equation (26)₄, are obtained using the equations outlined in Table 1 along with the thermodynamic potentials, Equations (39)–(41), and are listed in Table 3. These conjugates are linear relations in terms of their associated internal state variables due to the particular definition of Ψ^{tvp} and Ψ^{tvd} given by Equations (40) and (41), respectively.

A systematic way to show the dependency between the derived local state laws and the state laws associated with their Laplacian is outlined in the subsequent section.

The Nonlocal Conjugate Forces

As mentioned in the section on 'Viscoplasticity and Damage Internal State Variables', the assumed internal state variables in the current work are no longer independent and special care must be taken to properly account for state variable coupling between Ξ_n and $\nabla^2 \Xi_n$. Starting from Equation (5), the nonlocal evolution of $\widehat{\Xi}_n$ is written as follows (note that in all equations that follow, there is no sum in subscript n when n is repeated):

$$\stackrel{\nabla}{\Xi}_n = \dot{\Xi}_n + \frac{1}{2} l_n^2 \stackrel{\nabla}{\nabla^2} \Xi_n \qquad (n = 1, \dots, 4 \text{ and no sum in } n)$$
 (47)

such that

$$\dot{\hat{p}} = \dot{p} + \frac{1}{2}\ell_1^2 \nabla^{\nabla}_2 p; \qquad \dot{\hat{\alpha}}_{ij} = \overset{\nabla}{\alpha}_{ij} + \frac{1}{2}\ell_2^2 \nabla^{\nabla}_2 \alpha_{ij};
\dot{\hat{r}} = \dot{r} + \frac{1}{2}\ell_3^2 \nabla^{\nabla}_2 r; \qquad \dot{\hat{\Gamma}}_{ij} = \overset{\nabla}{\Gamma}_{ij} + \frac{1}{2}\ell_4^2 \nabla^{\nabla}_2 \Gamma_{ij}$$
(48)

In Equations (47) and (48), the gradient parameters ℓ_n $(n=1,\ldots,4)$ are length parameters required for dimensional consistency and they set the scales at which the gradients become important. They give rise to explicit length-scale measures. Even though a recent study by the current authors

(Abu Al-Rub and Voyiadjis, 2004; Voyiadjis and Abu Al-Rub, 2005) showed that the length-scale parameter changes with the microstructural features (e.g., grain size, dislocation spacing, etc.), the length-scale measures are treated as constants in this study. Moreover, Abu Al-Rub and Voyiadjis (2004) proposed that the gradient parameters ℓ_n ($n=1,\ldots,4$) must be calibrated from micromechanical tests where size effects and inelastic heterogeneity are encountered. Examples of such tests are micro-/nano-indentation tests (Stelmashenko et al., 1993), microbending tests (Stolken and Evans, 1998), and microtorsion tests (Fleck et al., 1994).

The evolution laws of Ξ_n (n = 1, ..., 4) and their corresponding Laplacian $\nabla^2 \Xi_n$ are given in Table 2. Following the equations listed in Table 3 for viscoplasticity and viscodamage hardening conjugate forces, we can express the evolution equations of the corresponding nonlocal conjugate forces at a given temperature as follows:

$$\hat{\Sigma}_{n} = c_{n} \hat{\Xi}_{n} \vartheta \quad (n = 1, \dots, 4 \text{ and no sum in } n)$$
(49)

where c_n $(n=1,\ldots,4)$ are material parameters that are characterized as hardening moduli. Moreover, \sum_n can be additively decomposed into two parts: one corresponding to the local counterpart of $\widehat{\Xi}_n$ and the other corresponding to the Laplacian counterpart, $\nabla^2\Xi_n$, such that (see Table 3):

$$\overset{\nabla}{\widehat{\Sigma}_n} = \overset{\nabla}{\Sigma_n} + \overset{\nabla}{\Sigma_n^g} \quad (n = 1, \dots, 4)$$
 (50)

Table 2. The thermodynamic laws for the evolution of the internal state variables.

| Plasticity Isotropic hardening Kinematic hardening | $\dot{oldsymbol{ ho}} = -\dot{\lambda}^{\mathrm{vp}} rac{\partial F}{\partial R} \ rac{\partial F}{lpha_{ij}} = -\dot{\lambda}^{\mathrm{vp}} rac{\partial F}{\partial X_{ij}}$ | $\nabla^{\nabla}_{2} \rho = -\nabla^{2} \dot{\lambda}^{vp} \partial_{R} F - \dot{\lambda}^{vp} \nabla^{2} \partial_{R} F$ $\nabla^{2} \alpha_{ij} = -\nabla^{2} \dot{\lambda}^{vp} \partial_{X} F - \dot{\lambda}^{vp} \nabla^{2} \partial_{X} F$ |
|--|---|---|
| Damage Isotropic hardening Kinematic hardening | $\dot{r} = -\dot{\lambda}^{ m vd} rac{\partial \mathbf{G}}{\partial \mathcal{K}} \ \Gamma_{ij}^{ abla} = -\dot{\lambda}^{ m vd} rac{\partial \mathbf{G}}{\partial H_{ij}}$ | $ abla^{ abla}_{ abla^{2}r} = - abla^{2}\dot{\lambda}^{\mathrm{vd}}\partial_{K}G - \dot{\lambda}^{\mathrm{vd}} abla^{2}\partial_{K}G $ $ abla^{ abla}_{ abla^{2}r} = - abla^{2}\dot{\lambda}^{\mathrm{vd}}\partial_{H}G - \dot{\lambda}^{\mathrm{vd}} abla^{2}\partial_{H}G $ |
| Damage variable | | $\nabla^{2} \overset{\nabla}{}_{(1)} \phi_{ij} = \nabla^{2} \dot{\lambda}^{vp} \partial_{y} f + \dot{\lambda}^{vp} \nabla^{2} \partial_{y} f$ $\nabla^{2} \dot{\lambda}^{vd} \partial_{y} g + \dot{\lambda}^{vd} \nabla^{2} \partial_{y} g$ |

Table 3. Expressions for the thermodynamic conjugate forces derived from the specific free-energy function.

| Plasticity Isotropic hardening Kinematic hardening | $R=a_1p_{artheta} \ X_{ij}=a_2lpha_{ij}artheta$ | $egin{aligned} R^{g} &= b_1 ig(abla^2 p ig) artheta \ X^{g}_{ij} &= b_2 ig(abla^2 lpha_{ij} ig) artheta \end{aligned}$ |
|--|--|---|
| Damage Isotropic hardening Kinematic hardening | $egin{aligned} \mathcal{K} &= \mathbf{a_3} r \vartheta \ \mathcal{H}_{ij} &= \mathbf{a_4} \Gamma_{ij} \vartheta \end{aligned}$ | $egin{aligned} \mathcal{K}^{	extsf{g}} &= b_3ig(abla^2 rig)artheta \ \mathcal{H}^{	extsf{g}}_{ij} &= b_4ig(abla^2 \Gamma_{ij}ig)artheta \end{aligned}$ |
| Damage force | $-Y_{ij} = \frac{\partial}{\partial \phi_{ij}} \begin{pmatrix} \mathbf{e}_{mn}^{\mathbf{e}} C_{mnpq} \mathbf{e}_{pq}^{\mathbf{e}} \\ -\beta_{mn} \mathbf{e}_{mn}^{\mathbf{e}} (T - T_{r}) \end{pmatrix}$ | $-Y_{ij}^{g} = \frac{\partial}{\partial \nabla^{2} \phi_{ij}} \begin{pmatrix} e_{mn}^{e} C_{mnpq} e_{pq}^{e} \\ -\beta_{mn} e_{mn}^{e} (T - T_{r}) \end{pmatrix}$ |

The conjugate forces $\overset{\nabla}{\Sigma}_n$ and $\overset{\nabla}{\Sigma}_n^g$ $(n=1,\ldots,4)$ are given at constant temperature, respectively, as follows (see Table 3):

$$\sum_{n=0}^{\nabla} a_n \stackrel{\nabla}{\Xi}_n \vartheta \qquad (n=1,\ldots,4 \text{ and no sum in } n)$$
 (51)

$$\sum_{n=0}^{\nabla} b_{n} \nabla^{2} \Xi_{n} \vartheta \qquad (n = 1, \dots, 4 \text{ and no sum in } n)$$
 (52)

However, substituting Equation (47) into Equation (49) yields:

$$\hat{\Sigma}_{n} = c_{n} \stackrel{\nabla}{\Xi}_{n} \vartheta + \frac{1}{2} c_{n} \ell_{n}^{2} \nabla^{2} \Xi_{n} \vartheta \quad (n = 1, \dots, 4 \text{ and no sum in } n)$$
 (53)

Comparing Equation (53) with Equations (50)–(52) yields:

$$\ell_n = \sqrt{\frac{2b_n}{a_n}}$$
 where $c_n = a_n$ $(n = 1, ..., 4)$ (54)

Taking the Laplacian of Equation (51) and neglecting temperature gradients we obtain:

$$\nabla^{\nabla} = a_n \nabla^{\nabla} \Xi_n \vartheta \qquad (n = 1, \dots, 4 \text{ and no sum in } n)$$
 (55)

Comparing the above equation with Equation (52) yields

$$\Sigma_n^{g} = \frac{b_n}{a_n} \nabla^{\nabla} \Sigma_n \qquad (n = 1, \dots, 4 \text{ and no sum in } n)$$
 (56)

Hence, Equation (50) can be rewritten as follows:

$$\widehat{\widehat{\Sigma}}_n = \widehat{\Sigma}_n^{\nabla} + \frac{b_n}{a_n} \nabla^2 \widehat{\Sigma}_n \qquad (n = 1, ..., 4 \text{ and no sum in } n)$$
 (57)

or substituting for b_n/a_n from Equation (54) we can rewrite the above equation as follows:

$$\widehat{\widehat{\Sigma}}_n = \widehat{\Sigma}_n^{\nabla} + \frac{1}{2} \ell_n^2 \nabla^2 \widehat{\Sigma}_n \qquad (n = 1, \dots, 4 \text{ and no sum in } n)$$
 (58)

which shows a similar relation to that of their corresponding fluxes given by Equation (47). The above results are summarized in Table 4.

The nonlocal evolution equation of the damage variable ϕ can also be written from Equation (5) as follows:

$$\widehat{\phi}_{ii}^{\nabla} = \widehat{\phi}_{ij} + a \nabla^{2} \widehat{\phi}_{ij}$$
 (59)

where $a=(1/2)\ell_5^2$ and the evolution equations of ϕ and $\nabla^2 \phi$ are given in Table 2. Using Equation (15) we then write:

$$\widehat{M}_{ikjl}^{-1} = M_{ikjl}^{-1} + a\nabla^2 M_{ikjl}^{-1}$$
 (60)

Table 4. The nonlocal thermodynamic laws and the corresponding length parameters at a given temperature.

| | Local | Gradient | Nonlocal | Length parameter |
|--------------------------------------|--|--|--|----------------------------|
| Plasticity Isotropic hardening | $\dot{R}=a_1\dot{p}\vartheta$ | $\dot{R}^{g} = b_1 \nabla^2 p \vartheta$ | V | $\ell_1 = \sqrt{2b_1/a_1}$ |
| Kinematic hardening | $\overset{V}{X_{ij}} = a_{2}\overset{\nabla}{\alpha_{ij}}\vartheta$ | $X_{ij}^{g} = b_2 \nabla^2 \alpha_{ij} \vartheta$ | $\hat{X}_{ij} = \hat{X}_{ij} + (1/2)\ell_2^2 \nabla^2 X_{ij}$ | $\ell_2 = \sqrt{2b_2/a_2}$ |
| Damage Isotropic hardening | $\dot{K}=a_3\dot{r}\vartheta$ | $\dot{K}^{\mathrm{g}}=b_{3} abla^{\mathrm{v}}r\vartheta$ | $\dot{\hat{K}} = \dot{K} + (1/2)\ell_3^2 \nabla^2 K$ | $\ell_3 = \sqrt{2b_3/a_3}$ |
| Kinematic hardening | $\overset{ abla}{H}_{ij}=a_{4}\overset{ abla}{\Gamma}_{ij}\vartheta$ | $H_{ij}^{g} = b_4 \nabla^2 \Gamma_{ij} \vartheta$ | $\hat{H}_{ij} = H_{ij}^{\nabla} + (1/2)\ell_4^2 \nabla^2 H_{ij}$ | $\ell_4 = \sqrt{2b_4/a_4}$ |

where

$$M_{ikjl}^{-1} = \frac{1}{2} \left[(\delta_{ik} - \phi_{ik}) \delta_{jl} + \delta_{ik} (\delta_{jl} - \phi_{jl}) \right] \quad \text{and} \quad \nabla^2 M_{ikjl}^{-1} = -\frac{1}{2} \left(\nabla^2 \phi_{ik} \delta_{jl} + \delta_{ik} \nabla^2 \phi_{jl} \right)$$

$$\tag{61}$$

Viscoplasticity and Viscodamage Potentials

The next important step in constitutive modeling is the selection of the appropriate form of the viscoplastic potential function F and the viscodamage potential function G to establish the desired constitutive equations. It is clearly seen in the previous sections that the viscodamage evolution laws are strongly coupled with viscoplasticity. To maintain this strong coupling, two independent damage mechanisms are distinguished. One mechanism is coupled with viscoplasticity, while the other is independent of the viscoplastic deformation. The first mechanism is dominant in the case of shear stresses and the second is due to hydrostatic stresses. To be consistent and to satisfy the generalized normality rule of thermodynamics, a proper analytical form for F and G need to be postulated in the undamaged configuration, such that:

$$F = f + \frac{1}{2}k_1\bar{\hat{R}}^2 + \frac{1}{2}k_2\bar{\hat{X}}_{ij}\bar{\hat{X}}_{ij} \quad \text{and} \quad G = g + \frac{1}{2}h_1\hat{K}^2 + \frac{1}{2}h_2\hat{H}_{ij}\hat{H}_{ij}$$
 (62)

where k_i and h_i (i = 1, 2) are material constants used to adjust the units of the terms comprising the above equations. The second-order tensor $\hat{X} = \bar{X} + \bar{X}^g$ is the nonlocal effective backstress tensor associated with the kinematic hardening and, analogous to Equation (8), can be related to its nominal part as follows:

$$\bar{\hat{X}}_{ij} = \hat{M}_{ikjl}\hat{X}_{kl} \quad \text{with} \quad \bar{X}_{ij} = \hat{M}_{ikjl}X_{kl} \quad \text{and} \quad \bar{X}_{ij}^{g} = \hat{M}_{ikjl}X_{kl}^{g}$$
(63)

The isotropic hardening/softening represents a global expansion/contraction in the size of the yield surface with no change in shape. Thus for a given yield criterion and flow rule, isotropic hardening/softening in any process can be predicted from the knowledge of the function $\hat{R} = \bar{R} + \bar{R}^g$ and this function may, in principle, be determined from a single test (e.g., the tension test). Therefore, the effective isotropic hardening functions \hat{R} , \hat{R} , and \hat{R}^g are related to the nominal isotropic hardening functions \hat{R} , \hat{R} , and \hat{R}^g , respectively, as follows:

$$\bar{\hat{R}} = \frac{\hat{R}}{1 - \hat{r}}, \quad \bar{R} = \frac{R}{1 - \hat{r}}, \quad \bar{R}^g = \frac{R^g}{1 - \hat{r}}$$
(64)

where \hat{r} is defined as the nonlocal accumulative viscodamage with \dot{r} given by Equation (38)₂, such that we express

$$\hat{r} = \int_0^t \dot{\hat{r}} \, \mathrm{d}t \quad \text{with} \quad \dot{\hat{r}} = \sqrt{\hat{\phi}_{ij}} \, \hat{\phi}_{ij}$$
 (65)

The derived flow rules, Equations (35) and (37), and the potential functions, Equations (62), indicate the need for two loading surfaces f and g. Thus, the coupled anisotropic viscodamage and viscoplasticity formulation is a two-surface model whereby anisotropic viscodamage is formulated in the spirit of viscoplasticity, complete with a viscodamage criterion and flow rules. It is possible, however, to activate one or both of the surfaces depending on the corresponding criteria for viscoplasticity and viscodamage.

VISCOPLASTICITY SURFACE AND THE CORRESPONDING HARDENING RULES

It seems natural that viscoplasticity can only affect the undamaged (effective) material skeleton. Therefore, the viscoplastic function f is defined in terms of the effective stresses and strains. There are many viscoplastic models in recent literature for dynamic material behavior at high strain rates and temperatures. A generalized dynamic surface, f, based on Perzyna unified viscoplasticity model can be utilized (Voyiadjis et al., 2003, 2004):

$$f = \sqrt{3J_2} - \left[\bar{Y}_0 + \hat{\bar{R}}\right] \left[1 + \left(\eta^{\text{vp}} \, \dot{\hat{p}}\right)^{1/m_1}\right] \vartheta \le 0 \tag{66}$$

where $J_2=1/2(\bar{\bf \tau}'-\hat{X}):(\bar{\bf \tau}'-\hat{X})$ is the second invariant of the resultant deviatoric stress tensor $(\bar{\bf \tau}'-\hat{X});\;\bar{\bf \tau}'$ is the effective deviatoric part of the Krichhoff stress tensor; \bar{Y}_0 is the initial yield stress in the undamaged state at zero absolute temperature, zero viscoplastic strain, and static strain rate; $\eta^{\rm vp}$ is the viscosity or fluidity parameter, which is referred to as the relaxation time according to the notation given by Perzyna (1988); $\hat{\bar{p}}$ is the nonlocal effective accumulative viscoplastic strain (see Equation (48)); m_1 is the viscoplastic rate sensitivity parameter; and $\vartheta=1-(T/T_{\rm m})$ is the homologous temperature.

The criterion in Equation (66) is a generalization of the classical rate-independent von-Mises yield criterion for rate-dependent materials. The latter can simply be recovered by imposing $\eta^{\rm vp} = 0$ (no viscosity effect), so that we have the case $f \le 0$. The extended criterion given by Equation (66) will play a crucial rule in the dynamic finite element formulation described

in the second part of this work. It also allows a generalization of the standard Kuhn-Tucker loading/unloading conditions (Voyiadjis et al., 2003, 2004):

$$f \le 0, \quad \dot{\lambda}^{\text{vp}} \ge 0, \quad \dot{\lambda}^{\text{vp}} f = 0$$
 (67)

with the generalized consistency condition for rate-dependent problems is given by:

$$\dot{\lambda}^{\mathrm{vp}}\dot{f} \equiv 0 \tag{68}$$

In Equation (66), f can expand and shrink not only by softening/hardening effects, but also due to softening/hardening rate effects. The right-hand side of Equation (66) defines the flow stress as a function of strain, strain-rate, and temperature and it converges to a great extent to the classical (local) constitutive laws of Johnson and Cook (1985), Zerilli and Armstrong (1987), and Voyiadjis and Abed (2005).

It is noteworthy that the adopted yield surface f, is a fully nonlocal surface, which is different from the nonlocal yield surfaces presented in the literature up to now. Most of these surfaces introduce nonlocality only through the isotropic hardening conjugate force, R (see e.g., de Borst and Sluys, 1991; Aifantis, 1992; Pamin, 1994; Fremond and Nedjar, 1996; Peerlings et al., 1996; Fleck and Hutchinson, 1997; Gao et al., 1999; Askes et al., 2000; Svedberg and Runesson, 2000; Liebe et al., 2003). Very few also introduce nonlocality through the kinematic hardening conjugate force, X (e.g., Voyiadjis et al., 2001, 2003, 2004). Both of the aforementioned approaches are quasi-nonlocal in a sense that a local quantity is added to a nonlocal quantity. In other words, for those who introduce nonlocality through R are adding to it a local part through J_2 , whereas for those who introduce nonlocality through X are adding to it a local part through τ' . However, in the current model, thanks to the effective (undamaged) configuration, nonlocality is introduced through R by \hat{p} and ϕ , through X by \hat{p} and ϕ , and through $\bar{\tau}'$ by ϕ .

The effective rate of the accumulative viscoplastic strain, \dot{p} , is defined by:

$$\dot{\bar{p}} = \sqrt{\frac{2}{3}} \, \bar{d}_{ij}^{\text{vp}} \bar{d}_{ij}^{\text{vp}} \tag{69}$$

where \bar{d}^{vp} is the viscoplastic strain rate in the effective configuration. Moreover, the energy-correlating hypothesis is adopted; each type of energy process in the damaged state is equal to corresponding to the effective configuration. Thus, \bar{d}^{vp} can be related to d^{vp} (Equation (35)₁)

through the use of the viscoplastic strain energy equivalence hypothesis (e.g., Lee et al., 1985; Voyiadjis and Thiagarajan, 1997; Voyiadjis and Deliktas, 2000), which states that the viscoplastic energy in terms of the effective and nominal stress and strain quantities must be equal. This gives the following relation, such that:

$$\bar{d}_{ij}^{\text{vp}} = \hat{M}_{ikjl}^{-1} d_{kl}^{\text{vp}} \tag{70}$$

Substituting Equation (35)₁ into Equation (70) and by making use of the effective stress definition (Equation (8)) and the chain rule, we can write \bar{d}^{vp} as follows:

$$\bar{d}_{ij}^{\text{vp}} = \dot{\lambda}^{\text{vp}} \frac{\partial f}{\partial \bar{\tau}_{ii}} \tag{71}$$

Since $(\partial f/\partial \bar{\tau}): (\partial f/\partial \bar{\tau}) = 1.5$, it can be easily shown that $\dot{\bar{p}}$ defined by Equation (69) is related to $\dot{\lambda}^{\rm vp}$ by:

$$\dot{\bar{p}} = \dot{\lambda}^{\text{vp}} \tag{72}$$

Substituting Equation $(62)_1$ into the evolution law of \dot{p} from Table 2, making use of the chain rule with Equation $(64)_2$, and finally comparing the result with Equation (72) yields the following expression:

$$\dot{p} = \frac{\dot{\bar{p}}}{1 - \hat{r}} \left(1 - k_1 \bar{\hat{R}} \right) \tag{73}$$

Note that in obtaining the above equation we set $(\partial f/\partial R) = -1$ since the evolution of R characterizes the radius of the yield surface in the absence of the strain rate effect. Moreover, by making use of the assumption of isotropy (i.e., neglecting the odd gradient terms) and neglecting higher-order terms, we obtain the following relation by either substituting Equation (64)₂ and λ^{vp} from Equation (72) into the definition of $\nabla^2 \dot{p}$ outlined in Table 2 or by simply taking the Laplacian of Equation (73), such that:

$$\nabla^2 \dot{p} = \left(\frac{\nabla^2 \dot{\bar{p}}}{1 - \hat{r}} + \frac{\nabla^2 r}{\left(1 - \hat{r}\right)^2} \dot{\bar{p}}\right) \left(1 - k_1 \bar{\hat{R}}\right) - \frac{\dot{\bar{p}}}{1 - \hat{r}} k_1 \nabla^2 \bar{R}$$
(74)

The term $\nabla^2 \bar{R}$ is obtained by substituting Equation (64)₂ into Equation (56), such that:

$$\nabla^2 \bar{R} = \frac{a_1}{b_1} \bar{R}^{g} + \frac{\nabla^2 r}{1 - \hat{r}} \bar{R}$$
 (75)

Making use of \vec{R} and \vec{R}^g relations from Table 4 together with the corotational derivative of Equations (64) for a given temperature while maintaining the damage history constant (i.e., the damage internal state variable ϕ and temperature T are kept constant) and substituting \vec{p} for \vec{p} from Equation (73) and $\nabla^2 \vec{p}$ for $\nabla^2 \vec{p}$ from Equation (74) along with Equation (75), we obtain the following evolution equations for \vec{R} and \vec{R}^g , respectively, as follows:

$$\dot{\bar{R}} = \frac{a_1 \vartheta}{\left(1 - \hat{r}\right)^2} \left(1 - k_1 \bar{\hat{R}}\right) \dot{\bar{p}} \tag{76}$$

$$\dot{\bar{R}}^{g} = S_{1}^{R}\dot{\bar{p}} + S_{2}^{R}\nabla^{2}\dot{\bar{p}} \tag{77}$$

where

$$S_{1}^{R} = \frac{\vartheta}{(1-\hat{r})^{3}} \left[b_{1} \left(1 - 2k_{1}\bar{R} - k_{1}\bar{R}^{g} \right) \nabla^{2}r - k_{1}a_{1} (1-\hat{r})\bar{R}^{g} \right] \quad \text{and}$$

$$S_{2}^{R} = \frac{b_{1}\vartheta}{(1-\hat{r})^{2}} \left(1 - k_{1}\bar{\hat{R}} \right)$$
(78)

The nonlocal evolution equation for the isotropic hardening in the effective configuration, \hat{R} , can then be written according to Equation (50) or from Table 4 as follows:

$$\dot{\hat{R}} = \dot{R} + \dot{R}^g \tag{79}$$

To derive the nonlocal kinematic hardening evolution equation associated with viscoplasticity, we make use of the evolution of α in Table 2 along with the chain rule and Equations (62)₂, (63)₂, (71), and (72) such that one can write the following relation:

$$\vec{\alpha}_{ij} = \hat{M}_{minj} \left(\bar{d}_{mn}^{vp} - k_2 \bar{\hat{X}}_{mn} \dot{\bar{p}} \right)$$
 (80)

However, using the \bar{X} relation in Table 4 and operating on the \bar{X} relation of Equation (63)₂ with the corotational derivative for a given temperature and keeping the damage history constant, we can write the following evolution equation for \bar{X} as follows:

$$\bar{\bar{X}}_{ij} = \hat{M}_{ikjl} \hat{M}_{mknl} \left(a_2 \bar{\bar{d}}_{mn}^{\text{vp}} - k_2 a_2 \dot{\bar{p}} \bar{\hat{X}}_{mn} \right) \vartheta$$
 (81)

Again, with the assumption of isotropy (i.e., neglecting the odd gradient terms) and neglecting higher-order terms, either by utilizing Equations (62), (71), and (72) into the evolution law of $\nabla^2 \alpha$ from Table 2 or by taking the Laplacian of Equation (80), the following expression can be obtained:

$$\nabla^{2} \overset{\nabla}{\alpha_{ij}^{v}} = \widehat{M}_{minj} \left[\nabla^{2} \bar{d}_{mn}^{vp} - k_{2} \left(\tilde{\widehat{X}}_{mn} \nabla^{2} \dot{\bar{p}} + \dot{\bar{p}} \nabla^{2} \bar{X}_{mn} \right) \right] + \nabla^{2} \widehat{M}_{minj} \left(\bar{d}_{mn}^{vp} - k_{2} \tilde{\widehat{X}}_{mn} \dot{\bar{p}} \right)$$
(82)

The term $\nabla^2 \bar{X}$ is obtained by substituting Equations (63) into Equation (56), such that:

$$\nabla^{2} \bar{X}_{ij} = \frac{a_{2}}{b_{2}} \bar{X}_{ij}^{g} - \hat{M}_{kilj} \nabla^{2} M_{krls}^{-1} \bar{X}_{rs}$$
 (83)

Making use of Equation (82) into the X^g relation from Table 4 along with Equation (83) and the corotational derivative of \bar{X}^g relation of Equation (63)₃ for a given temperature while keeping the damage history constant, we then write the gradient-dependent evolution equation of viscoplasticity kinematic hardening in the effective configuration, \bar{X}^g , as follows:

$$\bar{X}_{ij}^{\nabla} = {}^{(1)}\bar{X}_{ij}^{g} + {}^{(2)}\bar{X}_{ij}^{g}$$
(84)

$${}^{(1)}\bar{\bar{X}}_{ij}^{\mathrm{g}} = \hat{M}_{ikjl}\hat{M}_{mknl} \left[b_2 \nabla^2 \bar{\bar{d}}_{mn}^{\mathrm{vp}} - k_2 b_2 \bar{\hat{X}}_{mn} \nabla^2 \dot{\bar{p}} \right]$$

$$-k_2 \left(a_2 \bar{X}_{mn}^{g} - b_2 \widehat{M}_{pmqn} \nabla^2 M_{prqs}^{-1} \bar{X}_{rs} \right) \dot{\bar{p}} \right] \vartheta \qquad (85)$$

$${}^{(2)}\bar{\bar{X}}_{ij}^{g} = \hat{M}_{ikjl}\nabla^{2}\hat{M}_{mknl}\left(b_{2}\bar{\bar{d}}_{mn}^{vp} - k_{2}b_{2}\bar{\hat{X}}_{mn}\dot{\bar{p}}\right)\vartheta$$
(86)

$$\nabla^2 \bar{d}_{ij}^{\text{vp}} = \nabla^2 \dot{\bar{p}} \frac{\partial f}{\partial \bar{\tau}_{ij}}$$
 (87)

Note that since f = 0, Equations (84)–(87) are obtained by assuming that $\nabla^2(\partial_{\bar{\tau}}f) = \partial_{\bar{\tau}}(\nabla^2f) = 0$. This assumption implies that the considered point has yielded as well as the surrounding volume of a sphere of diameter ℓ_c (i.e., the length parameter) and there is no change in the flow direction with the position within ℓ_c .

By taking the Laplacian of the identity $\hat{M}: \hat{M}^{-1} = I$, we can write the following relation $\nabla^2 \hat{M}$ as it appears in Equation (86):

$$\nabla^2 \hat{M}_{ikjl} = -\hat{M}_{kmln} \hat{M}_{irjs} \nabla^2 M_{rmsn}^{-1}$$
(88)

The nonlocal evolution equation for kinematic hardening in the effective configuration, \hat{X} , can now be expressed according to Equation (50) or from Table 4 as follows:

$$\overset{\nabla}{\bar{X}}_{ij} = \overset{\nabla}{\bar{X}}_{ij} + \overset{\nabla}{\bar{X}}_{ij}^{g}$$
(89)

DAMAGE EVOLUTION CRITERION AND THE CORRESPONDING HARDENING RULES

The anisotropic viscodamage governing equations are viscoplasticity-like. Analogous to the dynamic viscoplastic surface presented in the previous section, a fully-nonlocal viscodamage surface g can then be simply assumed as follows:

$$g = \sqrt{(\hat{Y}_{ij} - \hat{H}_{ij})(\hat{Y}_{ij} - \hat{H}_{ij})} - [l_0 + \hat{K}][1 + (\eta^{\text{vd}} \dot{\hat{r}})^{1/m_2}]\vartheta \le 0$$
 (90)

where the nonlocal damage forces \hat{Y} and \hat{H} are, respectively, characterizing the viscodamage evolution and the viscodamage kinematic hardening laws; $l_{\rm o}$ is the initial damage threshold at zero absolute temperature, zero damage strain, and static strain rate; \hat{K} is the nonlocal damage isotropic hardening function; $\eta^{\rm vd}$ is the relaxation time that corresponds to the damage growth; and m_2 is the viscodamage rate sensitivity parameter. For generality, it is assumed here that the time-dependent behavior of both viscoplasticity and viscodamage mechanisms are controlled by different relaxation times associated with $\hat{\bar{p}}$ and \hat{r} , which may not generally be the case.

The above postulated dynamic viscodamage function g=0 is a generalization of the static (rate-independent) damage surface for rate-dependent materials. Similar to the viscoplastic surface, the static damage surface can be simply recovered by imposing $\eta^{\rm vd}=0$ (no viscous effect), so that we have the rate-independent damage case $g\leq 0$. The model response in the viscodamage domain is then characterized by the Kuhn–Tucker complementary conditions as follows:

$$g \le 0, \quad \dot{\lambda}^{\text{vd}} \ge 0, \quad \dot{\lambda}^{\text{vd}}g = 0$$
 (91)

and the damage generalized consistency condition for rate-dependent problems is given by:

$$\dot{\lambda}^{\text{vd}}\dot{\mathbf{g}} = 0 \tag{92}$$

To derive the hardening evolution equations associated with the viscodamage process, we follow the same procedure presented in the former section for viscoplasticity. By substituting Equation (62)₂ into the evolution law of \dot{r} from Table 2, the following relation is obtained:

$$\dot{r} = \dot{\lambda}^{\text{vd}} \left(1 - h_1 \hat{K} \right) \tag{93}$$

By taking the Laplacian of Equation (93) and making use of the assumption of isotropy, we obtain:

$$\nabla^2 \dot{r} = \nabla^2 \dot{\lambda}^{\text{vd}} \left(1 - h_1 \hat{K} \right) - h_1 \dot{\lambda}^{\text{vd}} \nabla^2 K \tag{94}$$

where $\nabla^2 K = a_3 K^g/b_3$ from Equation (56). The evolution equation for \hat{K} can be obtained by first making use of Equations (93) and (94) into \hat{K} and \hat{K}^g relations in Table 4 for a given temperature, such that the following expressions are obtained:

$$\dot{K} = a_3 \left(1 - h_1 \hat{K} \right) \dot{\lambda}^{\text{vd}} \vartheta \quad \text{and} \quad \dot{K}^{\text{g}} = \left[b_3 \left(1 - h_1 \hat{K} \right) \nabla^2 \dot{\lambda}^{\text{vd}} - h_1 a_3 K^{\text{g}} \dot{\lambda}^{\text{vd}} \right] \vartheta$$
(95)

The nonlocal evolution equation for the viscodamage isotropic hardening law, \hat{K} , can then be written according to Equation (50) or from Table 4 as follows:

$$\dot{\hat{K}} = \dot{K} + \dot{K}^{g} \tag{96}$$

Furthermore, the evolution equation for \hat{H} can be obtained by utilizing Equation (62)₂ into Γ and $\nabla^2\Gamma$ relations from Table 2 along with Equation (37)₂, such that:

$$\Gamma_{ij}^{\nabla} = {}^{(2)}\phi_{ij} - h_2\dot{\lambda}^{\mathrm{vd}}\hat{H}_{ij} \quad \text{and} \quad \nabla^2 \Gamma_{ij}^{\nabla} = \nabla^2 {}^{(2)}\phi_{ij} - h_2 \Big(\hat{H}_{ij}\nabla^2\dot{\lambda}^{\mathrm{vd}} + \dot{\lambda}^{\mathrm{vd}}\nabla^2 H_{ij}\Big)$$
(97)

where $\nabla^2 \mathbf{H} = a_4 \mathbf{H}^g/b_4$ from Equation (56). It can then be easily shown by utilizing, respectively, Equations (97) into \mathbf{H} and \mathbf{H}^g laws from Table 4

for a given temperature that the following evolution equations are obtained:

$$\overset{\nabla}{H_{ij}} = \left(a_4 \overset{\nabla}{}^{(2)} \phi_{ij} - h_2 a_4 \dot{\lambda}^{\text{vd}} \hat{H}_{ij} \right) \vartheta \quad \text{and}$$

$$\overset{\nabla}{H_{ij}^g} = \left[b_4 \overset{\nabla}{\nabla}^{2} \overset{\nabla}{}^{(2)} \dot{\phi}_{ij} - h_2 b_4 \hat{H}_{ij} \overset{\nabla}{\nabla}^2 \dot{\lambda}^{\text{vd}} - h_2 a_4 H_{ij}^g \dot{\lambda}^{\text{vd}} \right] \vartheta$$
(98)

where $\nabla^2 \stackrel{\nabla}{(2)} \phi = \nabla^2 \dot{\lambda}^{\text{vd}} \partial g / \partial Y$. The nonlocal evolution equation for the viscodamage kinematic hardening law, \hat{H} , can then be written according to Equation (50) or from Table 4 as follows:

$$\widehat{H}_{ij} = H_{ij} + H_{ij}^{\nabla}$$

$$(99)$$

Finally, to obtain the nonlocal viscodamage force, first the state laws Y and Y^g from Table 3 are expanded such that the following expressions are obtained after performing some lengthy algebraic manipulations:

$$Y_{ij} = \frac{1}{2} (\tau_{mn} - \beta_{mn} (T - T_{\rm r})) \hat{M}_{manb} J_{arbsij} \mathbb{C}_{rspq}^{-1} (\tau_{pq} + \beta_{pq} (T - T_{\rm r}))$$
(100)

$$Y_{ij}^{\mathbf{g}} = \frac{a}{2} (\tau_{mn} - \beta_{mn} (T - T_{\mathbf{r}})) \hat{M}_{manb} J_{arbsij} \mathbb{C}_{rspq}^{-1} (\tau_{pq} + \beta_{pq} (T - T_{\mathbf{r}}))$$
(101)

where J is a sixth-order constant tensor and is given by:

$$J_{arbsij} = -\frac{\partial \widehat{M}_{arbs}^{-1}}{\partial \phi_{ij}} = -a \frac{\partial \widehat{M}_{arbs}^{-1}}{\partial \nabla^2 \phi_{ij}} = -\frac{\partial \widehat{M}_{arbs}^{-1}}{\partial \widehat{\phi}_{ij}} = \frac{1}{2} \left(\delta_{ar} \, \delta_{bi} \, \delta_{sj} + \delta_{ai} \, \delta_{rj} \, \delta_{bs} \right)$$

$$(102)$$

Hence, the nonlocal viscodamage force is obtained as the sum of Equations (100) and (101), such that:

$$\hat{Y}_{ij} = \frac{(1+a)}{2} (\tau_{mn} - \beta_{mn} (T - T_{r})) \hat{M}_{manb} J_{arbsij} \mathbb{C}_{rspq}^{-1} (\tau_{pq} + \beta_{pq} (T - T_{r}))$$
 (103)

RATE-TYPE CONSTITUTIVE RELATION

Operating on the stress relation of Equation (43) with the corotational derivative yields:

$$\overset{\nabla}{\tau_{ij}} = \mathbb{C}_{ijkl} (d_{kl} - d_{kl}^{\text{vp}} - d_{kl}^{\text{vd}}) + \overset{\nabla}{\mathbb{C}_{ijkl}} e_{kl}^{\text{e}} - \beta_{ij} \dot{T} - \overset{\nabla}{\beta_{ij}} (T - T_{\text{r}})$$
(104)

where $\overset{\nabla}{\mathbb{C}}$ and $\overset{\nabla}{\pmb{\beta}}$ are given by

$$\overset{\nabla}{\mathbb{C}}_{ijkl} = \frac{\partial \mathbb{C}_{ijkl}}{\partial \widehat{M}_{abuv}^{-1}} \overset{\nabla}{\widehat{M}_{abuv}^{-1}} = \frac{\partial \mathbb{C}_{ijkl}}{\partial \widehat{M}_{abuv}^{-1}} \frac{\partial \widehat{M}_{abuv}^{-1}}{\partial \phi_{mn}} \overset{\nabla}{\phi_{mn}} \quad \text{and}$$

$$\overset{\nabla}{\beta}_{ij} = \frac{\partial \beta_{ij}}{\partial \widehat{M}_{abuv}^{-1}} \overset{\nabla}{\widehat{M}_{abuv}^{-1}} = \frac{\partial \beta_{ij}}{\partial \widehat{M}_{abuv}^{-1}} \frac{\partial \widehat{M}_{abuv}^{-1}}{\partial \phi_{mn}} \overset{\nabla}{\phi_{mn}}$$

$$(105)$$

Making use of Equations (10), (14), (44), and (102), we then obtain, after some lengthy algebraic manipulations and for a general thermo-hypoelasto-viscoplastic-viscodamage flow processes, the following relation:

$$\overset{\nabla}{\tau_{ij}} = \mathbb{C}_{ijkl} \left(d_{kl} - d_{kl}^{\text{vp}} - d_{kl}^{\text{vd}} \right) - A_{ijkl} \overset{\nabla}{\phi_{kl}} - \beta_{ij} \dot{T}$$
 (106)

where

$$A_{ijkl} = \left[-\frac{\partial \mathbb{C}_{ijmn}}{\partial \widehat{M}_{abuv}^{-1}} e_{mn}^{e} + \frac{\partial \beta_{ij}}{\partial \widehat{M}_{abuv}^{-1}} (T - T_{r}) \right] \frac{\partial \widehat{M}_{abuv}^{-1}}{\partial \phi_{kl}}$$

$$= J_{ibjvkl} \widehat{M}_{bpvq} \tau_{pq} + \mathbb{C}_{ijmn} \widehat{M}_{manu} \mathbb{C}_{bvrs}^{-1} (\tau_{rs} + \beta_{rs} (T - T_{r})) J_{abuvkl}$$
(107)

It is noteworthy that the above incremental stress–strain relation can be similarly found using the stress–strain relation in the effective configuration (Equation (44)). This equation shows that softening occurs due to the thermal and damage evolution.

THERMOMECHANICAL COUPLING

A local increase in temperature may influence the material behavior during deformation; necessitating the inclusion of temperature in the constitutive modeling of the material. Substituting the internal energy density e

$$e = \Psi + T\eta \tag{108}$$

into the first law of thermodynamics

$$\rho \dot{e} = \sigma_{ij} d_{ij} + \rho r_{\text{ext}} - \nabla_i q_i \tag{109}$$

yields the following energy balance equation

$$\rho(\dot{\Psi} + \eta \dot{T} + \dot{\eta}T) - \sigma_{ij}d_{ij} - \rho r_{\text{ext}} + \nabla_i q_i = 0$$
(110)

where $r_{\rm ext}$ is the density of external heat. Multiplying both sides of Equation (110) by $J=\rho_{\rm o}/\rho$ and substituting $\rho_{\rm o}\dot{\Psi}$ from Equation (27) into the resulting expression and taking into account Equation (46) yields the following relation:

$$\rho_{o}\dot{\boldsymbol{\eta}}T = \tau_{ij} \left(d_{ij}^{\text{vp}} + d_{ij}^{\text{vd}} \right) - J^{e}P d_{kk}^{e} - \Pi_{\text{int}} + \rho_{o} r_{\text{ext}}$$

$$+ \tilde{k}_{ij} \nabla_{i} T \nabla_{j} T + \frac{1}{T} \tilde{k}_{ij} \nabla_{i}^{\nabla} T \nabla_{j} T$$

$$(111)$$

where $\tilde{k}_{ij} = \rho_0 k_{ij}/\rho$. Making use of the definition for the specific entropy $\eta = \tilde{\eta}(\varepsilon^e, T, \aleph_k; k = 1, ..., 10)$, operating on the entropy relation, Equation (26)₂, with the corotational derivative and substituting the result into Equation (111) gives the thermomechanical heat balance equation as follows:

$$\rho_{o}c_{p}\dot{T} = \Upsilon \tau_{ij} \left(d_{ij}^{vp} + d_{ij}^{vd} \right) - J^{e}P d_{kk}^{e} + \sum_{k=3}^{10} \left(\frac{\partial \Sigma_{k}}{\partial T} T - \Sigma_{k} \right) \aleph_{k}^{\nabla}$$
$$- \beta_{ij} d_{ij}^{e} T + \rho r_{ext} + \tilde{k}_{ij} \nabla_{i} T \nabla_{j} T$$
(112)

In the above equation, $c_{\rm p}=T\partial\eta/\partial T$ is the tangent specific heat capacity at constant pressure which is used to approximate the specific heat capacity at constant stress, and Υ is the fraction of the viscoinelastic work rate converted to heat which is incorporated into the heat balance equation for more accurate comparisons with experiments.

The left-hand side of Equation (112) represents the total thermal dissipation. The first term on the right-hand side represents the rate of viscoinelastic work converted to heat; the second term represents the heat generation due to shock compression/dilatation-release; the third term represents the rate of internal heat generation that encompasses all dissipative processes excluding the gross viscoinelastic deformation that is present during viscoplastic and viscodamage deformation; the fourth term is the reversible thermoelastic effect; the fifth term represents an external heat source; and the last term is due to parabolic heat conduction. If the duration of the event is sufficiently short, the thermal conduction term becomes negligible, i.e., adiabatic conditions prevail.

FAILURE CRITERION

In this development, the failure criterion is based on the nonlocal evolution of the accumulated microdamage internal state variable, $\hat{\phi}$, and the equation of state for the thermodynamic pressure. It implies that for

$$\|\hat{\phi}\| = \sqrt{\hat{\phi}_{ij}\hat{\phi}_{ij}} = \|\phi\|_{c} \quad \text{and/or} \quad P = P_{\text{cutoff}}$$
 (113)

the material loses its carrying capacity, where $\|\phi\|_c$ is the critical damage when catastrophic failure in the material takes place and P_{cutoff} is the pressure cutoff value when tensile failure or compressive failure occurs. If either of the conditions in Equation (113) is satisfied, the stress field is assumed zero at the corresponding point. This describes the main feature observed experimentally that the load tends to zero at the fracture point.

CONCLUSIONS

We have presented in this article a general thermodynamic framework for the formulation of a coupled plastic-damage constitutive model for softening media in the finite strain range. This framework is based on the assumption of the nonlocal gradient-enhanced continua. A systematic construction of a hypoelasto-thermoviscoplastic and thermoviscodamage constitutive model destined for solving high velocity impact related problems is shown in detail. Thermodynamic consistency is restored through the derived constitutive equations to introduce and address issues, such as the statistical inhomogeneity in the evolution related viscoinelasticity state variables, and temperature, pressure, and strain-rate sensitivity. The interaction of length-scales is a crucial factor in understanding and controlling the distribution and size of the material defects, such as statistically stored and geometrically necessary dislocations, microvoids, and microcracks influence on the overall macroscopic response. In conclusion, this work has identified a framework leading to a physically motivated modeling of plastic-damage in materials. In addition, this context provides the proper multiscale treatment for the regularization of the localized failure of the material.

The proposed gradient approach introduces second-order gradients in the hardening variables (isotropic and kinematic) and in the damage variable. These higher-order gradients are considered physically and mathematically related to their local counterparts. Special care is used to properly

account for the coupling between the state variable and their corresponding higher-order gradients. However, the phenomenological nature of the proposed gradient-dependent theory leads to numerous material parameters, which are difficult to be fully determined based on the limited number of micromechanical, gradient-dominant experiments (such as microindentation, microbending, and microtorsion tests).

Length-scale parameters are implicitly and explicitly introduced into the present dynamical formalism. Implicit length-scale measure is introduced through the use of rate-dependent theory, while explicit length-scale measures are introduced through the use of nonlocal theory.

A detailed description of the computational aspects and numerical schemes for the integration of the resulting strongly coupled system of constitutive equations is presented in the companion article of Part II of this work.

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