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Gradient formulation in coupled damage-plasticity

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THIS WORK PROVIDES a consistent and systematic framework for the gradient approach in coupled damage-plasticity that enables one to better understand the effects of material inhomogeneity on the macroscopic behavior and the material instabilities. The idea of multiple scale effects is made more general and complete by introducing damage and plasticity internal state variables and the corresponding gradients at both the macro and mesoscale levels. The mesoscale gradient approach allows one to obtain more precise characterization of the nonlinearity in the damage distribution; to address issues such as lack of statistical homogeneous state variables at the macroscale level such as debonding of fibers in composite materials, crack, voids, etc., and to address nonlocal influences associated with crack interaction. The macroscale gradients allow one to address non-local behavior of materials and interpret the collective behavior of defects such as dislocations and cracks. The development of evolution equations for plasticity and damage is treated in a similar mathematical approach and formulation since both address defects such as dislocations for the former and cracks/voids for the latter. Computational issues of the gradient approach are introduced in a form that can be applied using the finite element approach.

1. Introduction

ENGINEERING MATERIALS contain defects that lead in some cases to specific pattern formation due to a coupling of inelastic mechanisms of microcrack and microvoid growth with plastic flow and fracture. Initially, loading of heterogeneous materials causes non-interacting microcracks and microvoids; however, experimental observations indicate that further loading will cause failure mechanisms to occur at localized zones of plasticity and damage where a lot of interaction and coalescence of microcracks and microvoids take place. These interactions lead to a degradation of the global stiffness and to a subsequent decrease of the load carrying capacity of the material. As damage localizes over a narrow region of the continuum, the characteristic length scale governing the variations of damage falls far below the scale of the state variables of strain and damage used to describe the response of the continuum. This leads to the case where the

wavelength of the damage distribution is predicted to be much smaller than the size of the material heterogeneities [1].

The classical local approach does not adequately capture a decreased length scale, and it is therefore necessary to look for alternative strategies for the solution of the problem such as micromechanical characterization, Cosserat continua, and nonlocal approaches. In the case of the nonlocal approach, a common procedure is to introduce the nonlocal terms either through an integral equation [2] or through a gradient equation [3].

Localization problems due to plasticity and damage can be handled by using the gradient approach at the macroscale. However, it is observed that for a given value of macroscopic damage variable variation, the macroscale response function associated with the representative volume elements (RVE) consisting of different distributions of defects are attributable to the differences in the size, orientation, and spatial distribution of defects within the RVEs. These are important factors that make the evolution function statistically inhomogeneous below the RVE scale. Macroscale strain and damage gradient approaches cannot capture this sub-representative volume element (SRVE) length-scale effect. Lacy *et. al.* [4] proposed a mesoscale gradient approach in order to obtain more precise characterization of the nonlinearity in the damage distribution, nonlocal influences associated with crack interaction, and statistical inhomogeneity of the evolution related damage variables.

Damage and plasticity internal state variables and the corresponding gradients at both the macro and mesoscale levels are introduced. By including both internal state variables of plasticity and damage, this work provides sufficient details of defects and their interaction to characterize physically the material behavior. By incorporating the gradient of these internal state variables, this work also addresses the non-local effects. The combined coupled concept of introducing gradients at the mesoscale and macroscale enables one to address two issues simultaneously. The mesoscale gradients allow one to address such issues as lack of statistical homogeneous state variables at the macroscale level such as debonding of fibers in composite materials, crack, voids, etc. On the other hand, the macroscale gradients allow one to address non-local behavior of materials and interpret the collective behavior of defects such as dislocations and cracks. This coupled proposed gradients formulation allows one to model size-dependent behavior of the materials together with localization.

2. Gradient model using non-local internal state variables

In order to introduce long-range microstructural interaction, the stress response at a material point is assumed to depend on the state of its neighborhood in addition to the state of the point itself. The use of nonlocal continua theory is

made in order to achieve that. KUHL *et. al.* [5] and MÜHLHAUS and AIFANTIS [6] have derived a gradient continuum enhancement as a special case of the general concept of nonlocal continua. At the position $\mathbf{x}$, the nonlocal tensor $\bar{\mathbf{A}}$ can be expressed as the weighted average of its local counterpart $\mathbf{A}$ over a surrounding volume V at a small distance $|\zeta| \leq L_c$ from $\mathbf{x}$ such that

$$\bar{\mathbf{A}} = \frac{1}{V} \int_V \mathbf{h}(\zeta)\mathbf{A}(\mathbf{x}+\zeta)dV \tag{2.1}$$

where L_c is an internal characteristic length [6] and $\mathbf{h}(\zeta)$ is a weight function that decays smoothly with distance and in this work is given by $\mathbf{h}(\zeta) = \mathbf{I}\,h(\zeta)$where $\mathbf{I}$ is an identity tensor. However, the identity tensor $\mathbf{I}$ may be suitably substituted by another tensor in order to induce further anisotropic behavior of the material.

The local tensor $\mathbf{A}$ in Eq. (2.1) can be approximated by a Taylor expansion at $\zeta = 0$ such that:

$$\mathbf{A}(\mathbf{x}+\zeta) = \mathbf{A}(\mathbf{x}) + \nabla\mathbf{A}(\mathbf{x})\zeta + \frac{1}{2!}\nabla^2\mathbf{A}(\mathbf{x})\zeta\zeta + \frac{1}{3!}\nabla^3\mathbf{A}(\mathbf{x})\zeta\zeta\zeta + \quad \ldots \quad . \tag{2.2}$$

where ∇^i denotes the i-th order gradient operator. Assuming only an isotropic influence of the averaging equation, the integrals of the odd terms in Eq. (2.2) vanish. Furthermore, making use of Eqs. (2.1) and (2.2) and truncating the TAYLOR series after the quadratic term, leads to the following expression for the nonlocal tensor $\bar{\mathbf{A}}$ [5]:

$$\bar{\mathbf{A}} = \frac{1}{V}\int_V h(\zeta)\mathbf{A}(\mathbf{x})\,dV + \frac{1}{2!V}\int_V h(\zeta)\nabla^2\mathbf{A}(\mathbf{x})\zeta\zeta\,dV. \tag{2.3}$$

This relation can be expressed as a partial differential equation such that [5]:

$$\bar{\mathbf{A}} = \mathbf{A} + \left(\frac{1}{2!V}\int_V [h(\zeta)]\zeta\zeta dV\right)\nabla^2\mathbf{A} = \mathbf{A} + a\nabla^2\mathbf{A} \tag{2.4}$$

where $\frac{1}{V}\int_V [h(\zeta)]dV = 1$. In Eq. (2.4), a is a constant proportional to a length squared and weights each component of the gradient term identically. If one assumes a more general tensorial character for $\mathbf{h}$ not necessarily confined to the expression in terms of an identity tensor, then one obtains a different weighting of the individual coefficients. This will give a weighting function with a tensorial nature a containing several different integration constants a_{ij}. We have thus introduced the gradient term $a\nabla^2\mathbf{A}$ as an approximation of the difference between the nonlocal tensor $\bar{\mathbf{A}}$ at $\mathbf{x}$ and the local tensor A at $\mathbf{x}$.

A similar expression for the non-local internal variable $\bar{\mathbf{A}}$ may be obtained at the mesoscale to characterize interface damage such as debonding of the fiber from the matrix such that $\bar{\hat{\mathbf{A}}} = \hat{\mathbf{A}} + a\hat{\nabla}^2\hat{\mathbf{A}}$. This allows one to describe $\bar{\hat{\mathbf{A}}}$ at a SRVE where the internal variable can only be statistically homogeneous at a subvolume of the RVE and $\hat{\nabla}^2\hat{\mathbf{A}}$ is its corresponding gradient.

3. Representative volume and sub-volume elements

The internal state variables are divided into two categories. The first category is statistically homogeneous at the RVE, while the second is statistically homogeneous at the SRVE. The definition of the RVE and SRVE is detailed in the work of NEMAT-NASSER and HORI [9].

In the literature, the RVE is the necessary minimum observation window that is used for the determination of the statistically homogenous elastic stiffness. The RVE is considered to be a cube with dimension L_{RVE} such that the following conditions are fulfilled:

$$\frac{d}{L_{RVE}} \ll 1, \qquad L_c \leq L_{RVE} \leq L, \qquad \left|\frac{\partial \sigma_{ij}^0}{\partial x_k}\right| L_{RVE} \ll |\sigma_{ij}^0|, \tag{3.1}$$

where d is a characteristic size of the micro-constituents, L_C is the heterogeneity correlation length, L is the characteristic macroscopic structural dimension, σ_{ij}^0 is the mean field stress and x_1, x_2, are x_3 the components of the Cartesian coordinates. The RVE implied in this work is the matrix with a single fiber in the middle of the RVE (Fig. 1).

The other category of internal state variables are those that can only be statistically homogenous at a subvolume of the RVE. For an RVE made of two

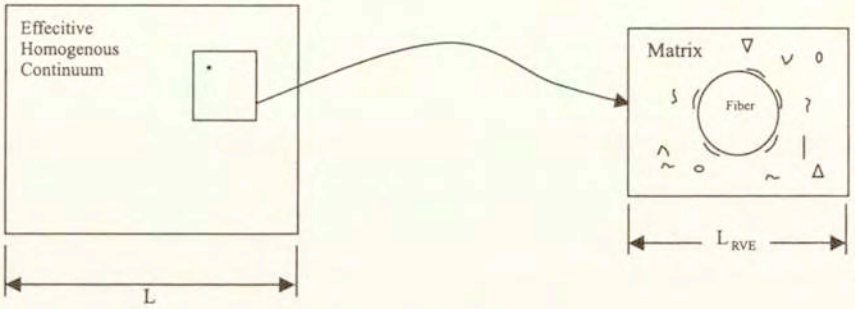

FIG. 1. Schematic representation of RVE

phase materials, the defect in each constituent and in the interphase (debonding) cannot be categorized as statistically homogenous for the RVE unless a very low order of measure of these defects is used to characterize damage or plasticity. The subvolume characterization of damage and plasticity at a level below the RVE allows one to adequately characterize the details of these defects. This SRVE definition for the composite material in the case of multi-scale analysis is introduced by defining an equivalent minimum observation window for each constituent of the composite where the response function of each constituent is statistically homogenous within the equivalent RVEs (Fig. 2). Then the sub-RVE damage distribution of each constituent can be characterized at a point within the corresponding RVEs.

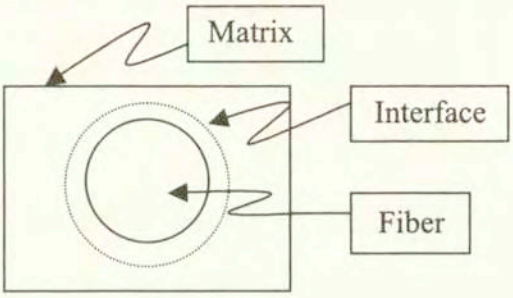

FIG. 2. Sub-RVEs for multiscale composite materials

4. Macroscale-mesoscale coupled plasticity and damage gradient theory using nonlocal internal state variables

The thermoelastic Helmoltz free energy may be expressed in terms of the nonlocal internal state variables as

$$(4.1)\quad \Psi = \Psi({}^{(e)}\varepsilon_{ij},\ T,\ {}^{(p)}\bar{\alpha}_{ij},\ {}^{(p)}\bar{p},\ {}^{(d)}\bar{\phi}_{ij}^{(u)},\ {}^{(d)}\bar{\gamma}_{ij},^{(u)},\ {}^{(d)}\bar{\kappa}^{(u)}) \quad \text{where } u = m, f, i,$$

where the subscribed letters after the variables indicate the tensorial nature of the variables. To the left of the variables, the bracketed superscript e implies elasticity-related internal state variable, p implies plasticity-related internal state variables, and d refers to the damage related internal state variables. The superscribed letter u to the right of the variables indicates that the different internal state variables are used to characterize the types of damages associated with the different material constituents. The composite material is divided into three components: matrix (m), fiber (f), and interface (i).

In the above equations, the nonlocal internal state variables $\bar{p}$ and $\bar{\alpha}_{ij}$ variables characterize the isotropic and kinematic hardening flux variables in plastic-

ity, respectively; the nonlocal internal state variables $\bar{\kappa}_{(u)}$ and $\bar{\gamma}_{ij}^{(u)}$ characterize the isotropic and kinematic hardening flux variables in damage, respectively. We define the kinematic hardening of the yield surface to be the cumulative effect from the flux-related backstresses. The $\bar{\phi}$ is the nonlocal damage second order tensor. Additive decomposition of the strain is assumed with $\varepsilon_{ij}^{'}$ being the elastic component and $\varepsilon_{ij}^{''}$ being the corresponding plastic component such that:

$$\varepsilon_{ij} = \varepsilon_{ij}^{'} + \varepsilon_{ij}^{''}. \tag{4.2}$$

The components of the macroscale gradient terms and the averaged mesoscale gradient terms of the macroscale internal state variables of both plasticity and damage may be used as additional higher order internal variables. In lieu of Section 1, with regard to using gradients to describe the non-local behavior of the material, the following relations are given here in a form similar to that given by Eqs. (5.1) and (5.2) such that:

$$\bar{\alpha}_{ij} = \alpha_{ij} + {}^{(p)}_{(2)}A\,\nabla^2\alpha_{ij} + {}^{(p)}_{(3)}A\,\widehat{\hat{\nabla}^2\hat{\alpha}_{ij}}, \tag{4.3}$$

$$\bar{p} = p + {}^{(p)}_{(2)}B\,\nabla^2 p + {}^{(p)}_{(3)}B\,\widehat{\hat{\nabla}^2\hat{p}}, \tag{4.4}$$

$$\bar{\gamma}_{ij}^{(u)} = \gamma_{ij}^{(u)} + {}^{(d)}_{(2)}A^{(u)}\ \nabla^2\gamma_{ij}^{(u)} + {}^{(d)}_{(3)}A^{(u)}\ \widehat{\hat{\nabla}^2\hat{\gamma}_{ij}^{(u)}}, \tag{4.5}$$

$$\bar{\kappa}^{(u)} = \kappa^{(u)} + {}^{(d)}_{(2)}B^{(u)}\ \nabla^2\kappa^{(u)} + {}^{(d)}_{(3)}B^{(u)}\ \widehat{\hat{\nabla}^2\hat{\kappa}^{(u)}}, \tag{4.6}$$

$$\bar{\phi}_{ij}^{(u)} = \phi_{ij}^{(u)} + {}^{(d)}_{(2)}C^{(u)}\ \nabla^2\phi_{ij}^{(u)} + {}^{(d)}_{(3)}C^{(u)}\ \widehat{\hat{\nabla}^2\hat{\phi}_{ij}^{(u)}}. \tag{4.7}$$

The constants ${}^{(p)}_{(r)}A$, ${}^{(p)}_{(r)}B$, ${}^{(d)}_{(r)}A^{(u)}$, ${}^{(d)}_{(r)}B^{(u)}$, and ${}^{(d)}_{(r)}C^{(u)}$ are constants similar to the constant a given by Eq. (2.4). If one chooses the same weight function $h(\zeta)$ for both the plasticity and damage macro-related internal variables, then one obtains

$${}^{(p)}_{(2)}A = {}^{(p)}_{(2)}B = {}^{(d)}_{(2)}A^{(u)} = {}^{(d)}_{(2)}B^{(u)} = {}^{(d)}_{(2)}C^{(u)} = A. \tag{4.8}$$

However, this will not be the case for the micro-related internal variables since the region of the sub-volume will change for different internal variables.

The isotropic hardening variable of plasticity, p, is a scalar quantity and is expressed in terms of the second order tensor, $\dot{\varepsilon}''_{ij}$ describing the plastic strain rate. The gradient terms of p characterize measures of the dislocation density [7]. The gradient terms referring to the backstress characterizes the internal embedded stress variations introduced by dislocation pile-ups, etc. The average mesoscale gradients of kinematic and isotropic hardening in plasticity may be used to characterize discrete dislocations in the formulation, if that is paramount to the analysis.

For the case of damage, the second order tensor, ϕ_{ij} characterizes a kinematic measure of damage due to volume or surface reduction associated with the evolution of voids or cracks, respectively [10-12]. The eigen values of define the Jacobian that describes the change in volume due to the micro-cracks and the micro-cavities. The damage is characterized through the individual damages of the matrix, $\phi_{ij}^{(m)}$ the fiber, $\phi_{ij}^{(f)}$ and the interface, $\phi_{ij}^{(i)}$ The gradients of the damages can also be used in this analysis. For the case of matrix damage, $\nabla^2\phi_{ij}^{(m)}$ is used, while for fiber damage,$\nabla^2\phi_{ij}^{(f)}$ is used. However, for the interface damage, the averaged mesoscale gradient $\widehat{\nabla^2\hat{\phi}_{ij}^{(i)}}$ is used which is averaged at the sub-volume of the RVE. The overall damage is obtained directly from VOYIADJIS and PARK [13].

The cohesive zone concept [14] applied to metal matrix composites is one of these processes that attempt to use evolution equations at the mesoscale and averaged at the macroscale level. To address the evolution behavior of such SRVE internal variables one must follow one of two approaches. The first and most robust one is to use evolution equations at the SRVE level to obtain the current state of characterization of these defects. These defects are then used to obtain gradients of these internal state variables that are averaged over a domain of subvolumes in order to recover the internal state variables at the macroscale. The alternative and more efficient but less precise approach is to integrate the evolution relations over the SRVE sectionally in order to obtain the evolution relations at the macroscale.

To simplify the formulations, a new notation for the internal state variables used in the Helmholtz free energy can be defined as follows [4]:

$$\underset{(1)}{\overset{(r)}{\mathbf{f}}} = \mathbf{f} = \frac{1}{V_{RVE}} \int_{V_{RVE}} \underset{(1)}{\overset{(r)}{\hat{\mathbf{f}}}} dV_{RVE} \tag{4.9}$$

$$\underset{(2)}{\overset{(r)}{\mathbf{f}}} = \nabla^2 \underset{(1)}{\overset{(r)}{\mathbf{f}}} \tag{4.10}$$

$$(4.11) \qquad {}^{(r)}_{(3)}\mathbf{f} = \widehat{\hat{\nabla}^2 {}^{(r)}_{(1)}\hat{\mathbf{f}}}$$

where the ${}^{(r)}_{(1)}\mathbf{f} = \mathbf{f}$ in these equations represent an RVE-averaged internal state variable evaluated using the macroscale coordinate system $\mathbf{x}$ and may be a tensor of any order. ${}^{(r)}_{(1)}\hat{\mathbf{f}}$ represents the local sub-RVE internal state variable evaluated using the mesoscale coordinate system $\hat{\mathbf{x}}$, and ${}^{(r)}_{(3)}\mathbf{f}$ represents an RVE average of a mesoscale internal state variable which measures the mesostructural variability within the RVE [4]. The gradient operators ∇ and $\hat{\nabla}$ involve spatial derivatives at the macroscale and mesoscale, respectively. The macroscale internal state variables given by Eq. (4.9) as well as the corresponding gradient terms given by Eqs. (4.10) and (4.11) are regarded as independent internal state variables with respect to each other. Consequently, independent evolution equations should be obtained with respect to each of these internal state variables that are subject to the appropriate boundary conditions for the corresponding internal state variable.

Incorporating the relations given by Eq. (4.8) - (4.11) into Eqs. (4.3) to (4.7) gives the following relations:

$$(4.12) \qquad \bar{\alpha}_{ij} = {}^{(p)}_{(1)}\alpha_{ij} + A^{(p)}_{(2)}\alpha_{ij} + {}^{(p)}_{(3)}A^{(p)}_{(3)}\alpha_{ij},$$

$$(4.13) \qquad \bar{p} = {}^{(p)}_{(1)}p + A^{(p)}_{(2)}p + {}^{(p)}_{(3)}B^{(p)}_{(3)}p,$$

$$(4.14) \qquad \bar{\gamma}^{(u)}_{ij} = {}^{(d)}_{(1)}\gamma^{(u)}_{ij} + A^{(d)}_{(2)}\gamma^{(u)}_{ij} + {}^{(d)}_{(3)}A^{(u)}{}^{(d)}_{(3)}\gamma^{(u)}_{ij},$$

$$(4.15) \qquad \bar{\kappa}^{(u)} = {}^{(d)}_{(1)}\kappa^{(u)} + A^{(d)}_{(2)}\kappa^{(u)} + {}^{(d)}_{(3)}B^{(u)}{}^{(d)}_{(3)}\kappa^{(u)},$$

$$(4.16) \qquad \bar{\phi}^{(u)}_{ij} = {}^{(d)}_{(1)}\phi^{(u)}_{ij} + A^{(d)}_{(2)}\phi^{(u)}_{ij} + {}^{(d)}_{(3)}C^{(u)}{}^{(d)}_{(3)}\phi^{(u)}_{ij}.$$

5. Macroscale-mesoscale coupled plasticity and damage gradient theory using local internal state variables

In this paper, the terms $\mathbf{A}$ and $\nabla^2\mathbf{A}$ given in Eq. (2.4) are regarded as two independent internal state variables with different physical interpretations and

initial conditions. This approach is used since certain internal variables such as the dislocation density expressed through $\nabla^2 p$ and the accumulated plastic strain, p, do not necessarily have the same evolution equation. They each have a different physical interpretation that guides one to use different evolution equations for $\nabla^2 p$ and p. Using the non-local internal variable $\bar{p}$ similar to Eq. (4.4) such that

$$\bar{p} = p + {}^{(p)}B\nabla^2 p, \tag{5.1}$$

will enforce both internal variables to have a single evolution expression. However, the term p is physically a macroscale measure obtained through the plastic strain rate while the term $\nabla^2 p$ is interpreted as a macroscale measure comparable to the mesoscale measure identified as the dislocation density [7]. This term maybe obtained computationally through the use of discrete dislocations and continuum plasticity. Similar arguments may be used for the flux-related back-stress plasticity tensor:

$$\bar{\alpha}_{ij} = \alpha_{ij} + {}^{(p)}A\nabla^2 \alpha_{ij}. \tag{5.2}$$

FLECK and HUTCHINSON [8] incorporated the measure of the average dislocation density into the flow strength. Allowing α_{ij} and $\nabla^2 \alpha_{ij}$ to be independent internal state variables instead of the single quantity $\bar{\alpha}_{ij}$ allows one to introduce computationally the independent macro and mesoscales. It also allows these two different physical phenomena to be identified separately with different evolution equations.

Equation (4.1) may now be expressed in terms of both the macroscale internal state variables and the averaged mesoscale gradients as

$$\Psi = \Psi({}^{(e)}\varepsilon_{ij}, T, {}^{(p)}_{(k)}\alpha_{ij}, {}^{(p)}_{(k)}p, {}^{(d)}_{(k)}\phi^{(u)}_{ij}, {}^{(d)}_{(k)}\gamma^{(u)}_{ij}, {}^{(d)}_{(k)}\kappa^{(u)}_{ij}), \quad k = 1, 2, 3. \tag{5.3}$$

We use Eq. (5.3) because Eq. (4.1) will lead to coupling terms of the nature $\alpha_{ij}\nabla^2(\alpha_{ij})$, etc. These coupling terms may not have a physical interpretation in material behavior. In this work, the authors do not introduce gradient effects directly through the strains and stresses by introducing terms such as $\bar{\varepsilon}_{ij}$ and $\bar{\sigma}_{ij}$. They are introduced only through the internal state variables associated with plasticity and damage. Stresses and strains are macro-variables that maybe computed using the macro-, meso-, and micro-structure internal state variables of the material.

Since the internal state variables are selected independently of one another, one can express the analytical form of the Helmholtz free energy given by Eq. (4.1) as the quadratic form in terms of its gradient-dependent internal state

variables as:

$$\rho\Psi = \frac{1}{2}\left(\varepsilon_{ij} - \varepsilon''_{ij}\right) E_{ijkl}\left(\varepsilon_{kl} - \varepsilon''_{kl}\right) + \sum_{k=1}^{3}\left(\frac{1}{2}{}^{(p)}_{(k)}a\,{}^{(p)}_{(k)}\alpha_{ij}\,{}^{(p)}_{(k)}b\,{}^{(p)}_{(k)}p\,{}^{(p)}_{(k)}p\right)$$

$$+ \sum_{u=m,f,i}\sum_{k=1}^{3}\left(\frac{1}{2}{}^{(d)}_{(k)}a^{(u)}\,{}^{(d)}_{(k)}\gamma^{(u)}_{ij}\,{}^{(d)}_{(k)}\gamma^{(u)}_{ij} + \frac{1}{2}{}^{(d)}_{(k)}b^{(u)}\,{}^{(d)}_{(k)}\kappa^{(u)}\,{}^{(d)}_{(k)}\kappa^{(u)}\right), \tag{5.4}$$

where the matrix $E_{ijkl} = E_{ijkl}\left(\bar{\phi}^{(u)}_{ij}\right)$ is the fourth-order damaged elastic stiffness tensor. In Eq. (5.4), the coefficients are dependent on material and geometrical properties of the composite. In the case of composites, the geometrical properties may include size, shape, and spacing of the fibers. In the case of the gradient theory these coefficients become also dependent on the gradient of the fiber size and fiber spacing variation. The functional dependence of these coefficients can be obtained by studying the interaction problem of an inclusion embedded in an infinite homogeneous matrix subjected to a macroscopic stress rate and the corresponding strain rate at infinity [7].

One can express the time derivative of Eq. (5.3) as follows:

$$\dot{\Psi} = \frac{\partial\Psi}{\partial\varepsilon'_{ij}}\dot{\varepsilon}'_{ij} + \frac{\partial\Psi}{\partial T}\dot{T} + \sum_{k=l}^{3}\left(\frac{\partial\Psi}{\partial^{(p)}_{(k)}\alpha_{ij}}\,{}^{(p)}_{(k)}\dot{\alpha}_{ij} + \frac{\partial\Psi}{\partial^{(p)}_{(k)}p}\,{}^{(p)}_{(k)}\dot{p}\right)$$

$$+ \sum_{u=m,f,i}\sum_{k=1}^{3}\left(\frac{\partial\Psi}{\partial^{(d)}_{(k)}\gamma^{(u)}_{ij}}\,{}^{(d)}_{(k)}\dot{\gamma}^{(u)}_{ij} + \frac{\partial\Psi}{\partial^{(d)}_{(k)}\kappa^{(u)}}\,{}^{(d)}_{(k)}\dot{\kappa}^{(u)} + \frac{\partial\Psi}{\partial^{(d)}_{(k)}\phi^{(u)}_{ij}}\,{}^{(d)}_{(k)}\dot{\phi}^{(u)}_{ij}\right). \tag{5.5}$$

By substituting of Eq. (5.5) into the Clausus-Duhem inequality one obtains

$$\left(\sigma_{ij} - \rho\frac{\partial\Psi}{\partial\varepsilon'_{ij}}\right)\dot{\varepsilon}'_{ij} - \rho\left(\frac{\partial\Psi}{\partial T} + s\right)\dot{T} + \sigma_{ij}\dot{\varepsilon}''_{ij} - \frac{q_{ij}}{T}\cdot\nabla T$$

$$- \sum_{k=1}^{3}\left(\rho\frac{\partial\Psi}{\partial^{(p)}_{(k)}\alpha_{ij}}\,{}^{(p)}_{(k)}\dot{\alpha}_{ij} + \rho\frac{\partial\Psi}{\partial^{(p)}_{(k)}p}\,{}^{(p)}_{(k)}\dot{p}\right)$$

$$- \sum_{u=m,f,i}\sum_{k=1}^{3}\left(\rho\frac{\partial\Psi}{\partial^{(d)}_{(k)}\gamma^{(u)}_{ij}}\,{}^{(d)}_{(k)}\dot{\gamma}^{(u)}_{ij} + \rho\frac{\partial\Psi}{\partial^{(d)}_{(k)}\kappa^{(u)}}\,{}^{(d)}_{(k)}\dot{\kappa}^{(u)} + \rho\frac{\partial\Psi}{\partial^{(d)}_{(k)}\phi^{(u)}_{ij}}\,{}^{(d)}_{(k)}\dot{\phi}^{(u)}_{ij}\right) \geq 0 \tag{5.6}$$

from which the thermodynamic state laws given in Table 1 are obtained. In this table, ${}^{(p)}_{(k)}X_{ij}$, ${}^{(p)}_{(k)}R$, ${}^{(d)}_{(k)}Y^{(u)}_{ij}$, ${}^{(p)}_{(k)}\Gamma^{(u)}_{ij}$, and ${}^{(d)}_{(k)}K^{(u)}$ are defined as the thermodynamic

conjugate forces corresponding to the internal state flux variables, respectively ${}^{(p)}_{(k)}\alpha_{ij}$, ${}^{(p)}_{(k)}p$, ${}^{(d)}_{(k)}\phi^{(u)}_{ij}$, ${}^{(d)}_{(k)}\gamma^{(u)}_{ij}$, and ${}^{(d)}_{(k)}\kappa^{(u)}$.

Using the equations in Table 1 along with Eq. (5.4), the definitions for the thermodynamic conjugate forces shown in Table 2 can be obtained.

Table 1. Thermodynamic State Laws

Thermoelastics Laws	Elastic deformation	$\sigma_{ij} = \rho\left(\partial\Psi/\partial\varepsilon'_{ij}\right)$
	Thermal entropy	$s = -\partial\Psi/\partial T$
Plasticity	Kinematic hardening	${}^{(p)}_{(k)}X_{ij} = \rho\left(\partial\Psi/\partial {}^{(p)}_{(k)}\alpha_{ij}\right)$
	Isotropic hardening	${}^{(p)}_{(k)}R = \rho\left(\partial\Psi/\partial {}^{(p)}_{(k)}p\right)$
Damage	Damage tensor	${}^{(d)}_{(k)}Y^{(u)}_{ij} = \rho\left(\partial\Psi/\partial {}^{(d)}_{(k)}\phi^{(u)}_{ij}\right)$
	Kinematic hardening	${}^{(d)}_{(k)}\Gamma^{(u)}_{ij} = \rho\left(\partial\Psi/\partial {}^{(d)}_{(k)}\gamma^{(u)}_{ij}\right)$
	Isotropic hardening	${}^{(d)}_{(k)}K^{(u)} = \rho\left(\partial\Psi/\partial {}^{(d)}_{(k)}\kappa^{(u)}\right)$

The value of the thermodynamic conjugate forces can be obtained through the evolution relations of the internal state variables. They are obtained by assuming the physical existence of the dissipation potential at the macroscale. With regard to the evolution equations for the averaged mesoscale based gradients, discrete elements, or micromechanical based models may be used to develop such relations.

The total power of dissipation can now be expressed as the sum of the plastic dissipation and damage dissipation as follows:

$$\Pi = \Pi^p + \Pi^d \tag{5.7}$$

where the dissipation processes are given as the sum of the products of the thermodynamic conjugate forces with the respective flux variables as follows:

$$\Pi^p = \sigma_{ij}\dot{\varepsilon}''_{ij} - \sum_{k=1}^{3}\left({}^{(p)}_{(k)}X_{ij}\ {}^{(p)}_{(k)}\dot{\alpha}_{ij} + {}^{(p)}_{(k)}R\ {}^{(p)}_{(k)}\dot{p}\right), \tag{5.8}$$

$$\Pi^d = -\sum_{u=m,f,i}\sum_{k=1}^{3}\left({}^{(d)}_{(k)}\Gamma^{(u)}_{ij}\ {}^{(d)}_{(k)}\dot{\gamma}^{(u)}_{ij} + {}^{(d)}_{(k)}K^{(u)}\ {}^{(d)}_{(k)}\dot{\kappa}^{(u)} + {}^{(d)}_{(k)}Y^{(u)}_{ij}\ {}^{(d)}_{(k)}\dot{\phi}^{(u)}_{ij}\right). \tag{5.9}$$

Table 2. Thermodynamic Conjugate Forces

Plasticity	Kinematic hardening	${}^{(p)}_{(k)}X_{ij} = {}^{(p)}_{(k)}a \; {}^{(p)}_{(k)}\alpha_{ij}$
	Isotropic hardening	${}^{(p)}_{(k)}R = {}^{(p)}_{(k)}b \; {}^{(p)}_{(k)}p$
Damage	Damage tensor	${}^{(d)}_{(k)}Y^{(u)}_{ij} = \frac{1}{2}\frac{\partial}{\partial\, {}^{(d)}_{(k)}\phi^{(u)}_{ij}}\left\{\left(\varepsilon_{ij} - \varepsilon''_{ij}\right)E_{ijkl}\left(\varepsilon_{kl} - \varepsilon''_{kl}\right)\right\}$
	Kinematic hardening	${}^{(d)}_{(k)}\Gamma^{(u)}_{ij} = {}^{(d)}_{(k)}a^{(u)} \; {}^{(d)}_{(k)}\gamma^{(u)}_{ij}$
	Isotropic hardening	${}^{(d)}_{(k)}K^{(u)} = {}^{(d)}_{(k)}b^{(u)} \; {}^{(d)}_{(k)}\kappa^{(u)}$

Since the plastic strain rate will be developed in the current deformed and damaged configuration, its corresponding evolution equation will be a function of the damage tensor. Similarly, the evolution equation of the conjugate force due to damage will be a function of the stress. The evolution equations for the plastic strain and the damage are interdependent [12], and therefore the two dissipative mechanisms shown above are implicitly interdependent through the stress and the conjugate forces due to damage.

The total power of dissipation can also be expressed by the sum of the dissipation mechanism due to plasticity and the dissipation mechanisms due to damage in each of the material constituents as follows:

$$\Pi = \Pi^{p} + \Pi^{d^{(m)}} + \Pi^{d^{(f)}} + \Pi^{d^{(i)}} \tag{5.10}$$

where the dissipation processes for each constituent are given as follows:

$$\Pi^{d^{(m)}} = -\sum_{k=1}^{3}\left({}^{(d)}_{(k)}\Gamma^{(m)}_{ij} \; {}^{(d)}_{(k)}\dot{\gamma}^{(m)}_{ij} + {}^{(d)}_{(k)}K^{(m)} \; {}^{(d)}_{(k)}\dot{\kappa}^{(m)} + {}^{(d)}_{(k)}Y^{(m)}_{ij} \; {}^{(d)}_{(k)}\dot{\phi}^{(m)}_{ij}\right), \tag{5.11}$$

$$\Pi^{d^{(f)}} = -\sum_{k=1}^{3}\left({}^{(d)}_{(k)}\Gamma^{(f)}_{ij} \; {}^{(d)}_{(k)}\dot{\gamma}^{(f)}_{ij} + {}^{(d)}_{(k)}K^{(f)} \; {}^{(d)}_{(k)}\dot{\kappa}^{(f)} + {}^{(d)}_{(k)}Y^{(f)}_{ij} \; {}^{(d)}_{(k)}\dot{\phi}^{(f)}_{ij}\right), \tag{5.12}$$

$$\Pi^{d^{(i)}} = -\sum_{k=1}^{3}\left({}^{(d)}_{(k)}\Gamma^{(i)}_{ij} \; {}^{(d)}_{(k)}\dot{\gamma}^{(i)}_{ij} + {}^{(d)}_{(k)}K^{(i)} \; {}^{(d)}_{(k)}\dot{\kappa}^{(i)} + {}^{(d)}_{(k)}Y^{(i)}_{ij} \; {}^{(d)}_{(k)}\dot{\phi}^{(i)}_{ij}\right). \tag{5.13}$$

The dissipation potentials of the damage in each of the constituents are interdependent through dependence of the damage tensors on the stress.

In this work, the evolution equations of the macroscale internal state variables are obtained through the use of the generalized normality rule of thermodynamics. In this regard the macroscale dissipation potential is defined in terms of the gradient-dependent internal state variables as a continuous and convex scalar-valued function of the flux variables [12]:

$$\Theta = \Theta\Big(\dot{\varepsilon}''_{ij},\ T,\ {}^{(p)}_{(k)}\dot{\alpha}_{ij},\ {}^{(p)}_{(k)}\dot{p},\ {}^{(p)}_{(k)}\dot{\phi}^{(u)}_{ij},\ {}^{(p)}_{(k)}\dot{\gamma}^{(u)}_{ij},\ {}^{(p)}_{(k)}\dot{\kappa}^{(u)}\Big). \tag{5.14}$$

By using the Legendre-Fenchel transformation of the dissipation potential $\Theta^{(u)}$, one can obtain complementary laws in the form of the evolution laws of flux variables as functions of the dual variables which can be decoupled into the plastic and damage dissipation potential parts as follows:

$$\begin{aligned}\Theta^* &= \Theta^*\Big(\sigma_{ij}, {}^{(p)}_{(k)}X_{ij}, {}^{(p)}_{(k)}R, {}^{(d)}_{(k)}Y^{(u)}_{ij}, {}^{(d)}_{(k)}K^{(u)}, {}^{(d)}_{(k)}\Gamma^{(u)}_{ij}\Big) \\ &= F\Big(\sigma_{ij}, {}^{(p)}_{(k)}R, {}^{(p)}_{(k)}X_{ij}\Big) + \sum_{m,f,i} G^{(u)}\Big({}^{(d)}_{(k)}Y^{(u)}_{ij}, {}^{(d)}_{(k)}K^{(u)}, {}^{(d)}_{(k)}\Gamma^{(u)}_{ij}\Big).\end{aligned} \tag{5.15}$$

As noted previously for the dissipation mechanisms, there is an implicit coupling between the plastic and damage dissipation potentials through the stress and the conjugate damage force.

6. Gradient-dependent thermodynamic conjugate forces

Assuming a similar definition for the nonlocal conjugate forces as for the conjugate forces given in Table 2, one obtains the following relations:

$$\bar{X}_{ij} = {}^{(p)}\bar{a}\,\bar{\alpha}_{ij} = {}^{(p)}\bar{a}\Big(\alpha_{ij} + A\nabla^2\alpha_{ij} + {}^{(p)}_{(3)}A\,\widehat{\hat{\nabla}^2\hat{\alpha}_{ij}}\Big), \tag{6.1}$$

$$\bar{R} = {}^{(p)}\bar{b}\,\bar{p} = {}^{(p)}\bar{b}\Big(p + A\,\nabla^2 p + {}^{(p)}_{(3)}B\,\widehat{\hat{\nabla}^2\hat{p}}\Big), \tag{6.2}$$

$$\bar{\Gamma}^{(u)}_{ij} = {}^{(d)}\bar{a}^{(u)}\,\bar{\gamma}^{(u)}_{ij} = {}^{(d)}\bar{a}^{(u)}\Big(\gamma^{(u)}_{ij} + A\,\nabla^2\gamma^{(u)}_{ij} + {}^{(d)}_{(3)}A^{(u)}\,\widehat{\hat{\nabla}^2\hat{\gamma}^{(u)}_{ij}}\Big), \tag{6.3}$$

$$\bar{K}^{(u)} = {}^{(d)}\bar{b}^{(u)}\bar{\kappa}^{(u)} = {}^{(d)}\bar{b}^{(u)}\Big(\kappa^{(u)} + A\,\nabla^2\kappa^{(u)} + {}^{(d)}_{(3)}B^{(u)}\,\widehat{\hat{\nabla}^2\hat{\kappa}^{(u)}}\Big). \tag{6.4}$$

One now makes use of the relations in Table 2 to obtain

$$\bar{X}_{ij} = {}^{(p)}_{(1)}\tilde{A}\,{}^{(p)}_{(1)}X_{ij} + {}^{(p)}_{(2)}\tilde{A}\,{}^{(p)}_{(2)}X_{ij} + {}^{(p)}_{(3)}\tilde{A}\,{}^{(p)}_{(3)}X_{ij}, \tag{6.5}$$

$$\bar{R} = {}^{(p)}_{(1)}\tilde{B}\,{}^{(p)}_{(1)}R + {}^{(p)}_{(2)}\tilde{B}\,{}^{(p)}_{(2)}R + {}^{(p)}_{(3)}\tilde{B}\,{}^{(p)}_{(3)}R, \tag{6.6}$$

$$\bar{\Gamma}^{(u)}_{ij} = {}^{(d)}_{(1)}\tilde{A}^{(u)}\,{}^{(d)}_{(1)}\Gamma^{(u)}_{ij} + {}^{(d)}_{(2)}\tilde{A}^{(u)}\,{}^{(d)}_{(2)}\Gamma^{(u)}_{ij} + {}^{(d)}_{(3)}\tilde{A}^{(u)}\,{}^{(d)}_{(3)}\Gamma^{(u)}_{ij}, \tag{6.7}$$

$$\bar{K}^{(u)} = {}^{(d)}_{(1)}\tilde{B}^{(u)}\,{}^{(d)}_{(1)}K^{(u)} + {}^{(d)}_{(2)}\tilde{B}^{(u)}\,{}^{(d)}_{(2)}K^{(u)} + {}^{(d)}_{(3)}\tilde{B}^{(u)}\,{}^{(d)}_{(3)}K^{(u)}, \tag{6.8}$$

where the constants are given by

$${}^{(r)}_{(k)}\tilde{A} = {}^{(r)}\bar{a}\frac{{}^{(r)}_{(k)}A}{{}^{(r)}_{(k)}a} \qquad \left({}^{(r)}_{(1)}A = 1,\ {}^{(r)}_{(2)}A = A\right), \tag{6.9}$$

$${}^{(r)}_{(k)}\tilde{B} = {}^{(r)}\bar{b}\frac{{}^{(r)}_{(k)}B}{{}^{(r)}_{(k)}b} \qquad \left({}^{(r)}_{(1)}B = 1,\ {}^{(r)}_{(2)}B = A\right). \tag{6.10}$$

In the above equations, $r = d$ for damage and $r = p$ for plasticity.

Here it is assumed that the relationship between the nonlocal thermodynamic force for damage and the nonlocal damage tensor is a linear relationship in the same form as Eqs. (6.1) to (6.4), which gives the following equations:

$$\bar{Y}^{(u)}_{ij} = {}^{(d)}\bar{c}\,\bar{\phi}^{(u)}_{ij} = {}^{(d)}\bar{c}\left(\phi^{(u)}_{ij} + A\,\nabla^2\phi^{(u)}_{ij} + {}^{(p)}_{(3)}A\,\hat{\bar{\nabla}}^2\,\hat{\phi}^{(u)}_{ij}\right), \tag{6.11}$$

$$\bar{Y}^{(u)}_{ij} = {}^{(d)}_{(1)}\tilde{C}^{(u)}\,{}^{(d)}_{(1)}Y^{(u)}_{ij} + {}^{(d)}_{(2)}\tilde{C}^{(u)}\,{}^{(d)}_{(2)}Y^{(u)}_{ij} + {}^{(d)}_{(3)}\tilde{C}^{(u)}\,{}^{(d)}_{(3)}Y^{(u)}_{ij}, \tag{6.12}$$

where the constants are given by

$${}^{(d)}_{(k)}\tilde{C} = {}^{(d)}\bar{c}\frac{{}^{(d)}_{(k)}C}{{}^{(d)}_{(k)}c} \qquad \left({}^{(d)}_{(1)}C = 1,\ {}^{(d)}_{(2)}C = A\right). \tag{6.13}$$

7. Evolution equations for the internal state variables

The theory of functions of several variables is used with the Lagrange multipliers $\dot{\lambda}_p$ and $\dot{\lambda}_d$ to construct the objective function Ω in the following form:

The theory of functions of several variables is used with the Lagrange multipliers and to construct the objective function in the following form:

$$\Omega = \Pi^p + \Pi^{d^{(m)}} + \Pi^{d^{(f)}} + \Pi^{d^{(i)}} - \dot{\lambda}_p F - \dot{\lambda}_d \left(G^{(m)} + G^{(f)} + G^{(i)}\right) \tag{7.1}$$

where F and $G^{(u)}$ are plastic and damage potential functions, respectively, and will be defined in subsequent sections. In order to obtain the plastic strain rate and the damage rate, the following conditions are used to extremize the objective function:

$$\frac{\partial \Omega}{\partial \sigma} = 0, \tag{7.2}$$

$$\frac{\partial \Omega}{\partial^{(d)}_{(k)} Y^{(u)}_{ij}} = 0. \tag{7.3}$$

From these conditions for the case when $F \geq 0$ and $G^{(u)} \geq 0$, the corresponding coupled evolution equations for the plastic strain and the damage are given as:

$$\dot{\varepsilon}''_{ij} = \dot{\lambda}_p \frac{\partial F}{\partial \sigma_{ij}} + \dot{\lambda}_d \left(\frac{\partial G^{(m)}}{\partial \sigma_{ij}} + \frac{\partial G^{(f)}}{\partial \sigma_{ij}} + \frac{\partial G^{(i)}}{\partial \sigma_{ij}} \right), \tag{7.4}$$

$$\overset{(d)}{(1)}\dot{\phi}^{(u)}_{ij} = -\dot{\lambda}_p \frac{\partial F}{\partial^{(d)}_{(1)} Y^{(u)}_{ij}} - \dot{\lambda}_d \frac{\partial G^{(u)}}{\partial^{(d)}_{(1)} Y^{(u)}_{ij}} = \overset{(d)}{(1)}\tilde{C}^{(u)} \left(-\dot{\lambda}_p \frac{\partial F}{\partial \bar{Y}^{(u)}_{ij}} - \dot{\lambda}_d \frac{\partial G^{(u)}}{\partial \bar{Y}^{(u)}_{ij}} \right), \tag{7.5}$$

$$\overset{(d)}{(2)}\dot{\phi}^{(u)}_{ij} = -\dot{\lambda}_p \frac{\partial F}{\partial^{(d)}_{(2)} Y^{(u)}_{ij}} - \dot{\lambda}_d \frac{\partial G^{(u)}}{\partial^{(d)}_{(2)} Y^{(u)}_{ij}} = \overset{(d)}{(2)}\tilde{C}^{(u)} \left(-\dot{\lambda}_p \frac{\partial F}{\partial \bar{Y}^{(u)}_{ij}} - \dot{\lambda}_d \frac{\partial G^{(u)}}{\partial \bar{Y}^{(u)}_{ij}} \right), \tag{7.6}$$

$$\overset{(d)}{(3)}\dot{\phi}^{(u)}_{ij} = -\dot{\lambda}_p \frac{\partial F}{\partial^{(d)}_{(3)} Y^{(u)}_{ij}} - \dot{\lambda}_d \frac{\partial G^{(u)}}{\partial^{(d)}_{(3)} Y^{(u)}_{ij}} = \overset{(d)}{(3)}\tilde{C}^{(u)} \left(-\dot{\lambda}_p \frac{\partial F}{\partial \bar{Y}^{(u)}_{ij}} - \dot{\lambda}_d \frac{\partial G^{(u)}}{\partial \bar{Y}^{(u)}_{ij}} \right). \tag{7.7}$$

However, plastic strain is assumed to occur only in the matrix. Therefore, the evolution of the plastic strain given by Eq. (7.4) is reduced to:

$$\dot{\varepsilon}''_{ij} = \dot{\lambda}_p \frac{\partial F}{\partial \sigma_{ij}} + \dot{\lambda}_d \frac{\partial G^{(m)}}{\partial \sigma_{ij}}. \tag{7.8}$$

However, one can still use Eq. (7.4) by insisting that fiber damage and damage due to debonding can produce permanent non-recoverable strains that should be added to the plastic strain.

Taking the time derivative of the definition for the non-local damage tensor $\bar{\phi}^{(u)}_{ij}$ given by Eq. (4.15) results in the following formula:

$$\dot{\bar{\phi}}^{(u)}_{ij} = \overset{(d)}{(1)}\dot{\phi}^{(u)}_{ij} + A \overset{(d)}{(2)}\dot{\phi}^{(u)}_{ij} + \overset{(d)}{(3)}C^{(u)} \overset{(d)}{(3)}\dot{\phi}^{(u)}_{ij}. \tag{7.9}$$

Substitution of Eqs. (7.5) to (7.7) into this equation gives the evolution of the damage tensor as:

$$\begin{aligned} \dot{\bar{\phi}}^{(u)}_{ij} = &-\dot{\lambda}_p \left(\frac{\partial F}{\partial \overset{(d)}{(1)}Y^{(u)}_{ij}} + A \frac{\partial F}{\partial \overset{(d)}{(2)}Y^{(u)}_{ij}} + \overset{(d)}{(3)}C^{(u)} \frac{\partial F}{\partial \overset{(d)}{(3)}Y^{(u)}_{ij}} \right) \\ &- \dot{\lambda}_d \left(\frac{\partial G^{(u)}}{\partial \overset{(d)}{(1)}Y^{(u)}_{ij}} + A \frac{\partial G^{(u)}}{\partial \overset{(d)}{(2)}Y^{(u)}_{ij}} + \overset{(d)}{(3)}C^{(u)} \frac{\partial G^{(u)}}{\partial \overset{(d)}{(3)}Y^{(u)}_{ij}} \right) \end{aligned} \tag{7.10}$$

which from Eq. (6.12) becomes:

$$\dot{\bar{\phi}}^{(u)}_{ij} = -\left(\dot{\lambda}_p \frac{\partial f}{\partial \bar{Y}^{(u)}_{ij}} + \dot{\lambda}_d \frac{\partial g^{(u)}}{\partial \bar{Y}^{(u)}_{ij}} \right) \left(\overset{(d)}{(1)}\tilde{C}^{(u)} + A \overset{(d)}{(2)}\tilde{C}^{(u)} + \overset{(d)}{(3)}C^{(u)} \overset{(d)}{(3)}\tilde{C}^{(u)} \right). \tag{7.11}$$

Coupling occurs between the evolution equations of the damage tensor and plastic strain due to the dependence of σ_{ij} on $\bar{\phi}^{(u)}_{ij}$ and $\bar{Y}^{(u)}_{ij}$ on σ_{ij}. It can be seen that if $F \leq 0$ or, $G^{(u)} \leq 0$, the evolution equations for the plastic strain and the damage will become decoupled [12].

7.1. Thermodynamic Potential of Plasticity and Yield Criterion

In order to obtain evolution equations for the internal state variables, a proper analytical form of the potentials that are defined in Eq. (5.15) needs to be obtained. In order to satisfy the generalized normality rule of thermodynamics, the following form of the plastic potential function, F, is defined here:

$$F = f + \frac{k_p}{2} \bar{X}_{ij} \bar{X}_{ij}. \tag{7.12}$$

In Eq. (7.12), k_p is a constant used to adjust the units of the equation, and f is the yield function and can be defined such that

$$f = \left\{ \frac{3}{2}(s_{ij} - \bar{X}_{ij})(s_{ij} - \bar{X}_{ij}) \right\}^{1/2} - \left[\sigma_{yp} + \bar{R} \right] \equiv 0 \tag{7.13}$$

in terms of the non-local conjugate forces $\bar{X}_{ij}$ and $\bar{R}$ where is the deviatoric component of the stress tensor σ_{ij}.

Gradient-dependent evolution equations of the internal state variables for plasticity can be obtained using the generalized normality rule of thermodynamics along with Eqs. (7.12) and (7.13)

$$\overset{(p)}{(1)}\dot{\alpha}_{ij} = -\dot{\lambda}_p \frac{\partial F}{\partial \overset{(p)}{(1)}X_{ij}} = -\dot{\lambda}_p \overset{(p)}{(1)}\tilde{A} \left\{ \frac{\partial f}{\partial \bar{X}_{ij}} + k_p \bar{X}_{ij} \right\}, \tag{7.14}$$

$$\overset{(p)}{(2)}\dot{\alpha}_{ij} = -\dot{\lambda}_p \frac{\partial F}{\partial \overset{(p)}{(2)}X_{ij}} = -\dot{\lambda}_p \overset{(p)}{(2)}\tilde{A} \left\{ \frac{\partial f}{\partial \bar{X}_{ij}} + k_p \bar{X}_{ij} \right\}, \tag{7.15}$$

$$\overset{(p)}{(3)}\dot{\alpha}_{ij} = -\dot{\lambda}_p \frac{\partial F}{\partial \overset{(p)}{(3)}X_{ij}} = -\dot{\lambda}_p \overset{(p)}{(3)}\tilde{A} \left\{ \frac{\partial f}{\partial \bar{X}_{ij}} + k_p \bar{X}_{ij} \right\}, \tag{7.16}$$

$$\overset{(p)}{(1)}\dot{p} = -\dot{\lambda}_p \frac{\partial F}{\partial \overset{(p)}{(1)}R} = -\dot{\lambda}_p \overset{(p)}{(1)}\tilde{B} \frac{\partial f}{\partial \bar{R}} = \dot{\lambda}_p \overset{(p)}{(1)}\tilde{B}, \tag{7.17}$$

$$\overset{(p)}{(2)}\dot{p} = -\dot{\lambda}_p \frac{\partial F}{\partial \overset{(p)}{(2)}R} = -\dot{\lambda}_p \overset{(p)}{(2)}\tilde{B} \frac{\partial f}{\partial \bar{R}} = \dot{\lambda}_p \overset{(p)}{(2)}\tilde{B}, \tag{7.18}$$

$$\overset{(p)}{(3)}\dot{p} = -\dot{\lambda}_p \frac{\partial F}{\partial \overset{(p)}{(3)}R} = -\dot{\lambda}_p \overset{(p)}{(3)}\tilde{B} \frac{\partial f}{\partial \bar{R}} = \dot{\lambda}_p \overset{(p)}{(3)}\tilde{B}. \tag{7.19}$$

An alternate approach to evolution Eqs. (7.15) and (7.16) is to obtain an evolution equation for α_{ij} only using the potential, F, as indicated by Eq. (7.12). The evolution equation for the corresponding gradient term of α_{ij} specifically, $\nabla^2\dot{\alpha}_{ij}$, is to be obtained directly by operating on $\dot{\alpha}_{ij}$ with the laplacian. An evolution equation for the averaged mesoscale gradient term, $\overline{\hat{\nabla}^2\hat{\alpha}_{ij}}$, is to be derived

at the mesoscale level using $\hat{\alpha}_{ij}$ through crystal plasticity, etc. and averaged over the RVE instead of Eq. (7.16). The same arguments apply for the subsequent evolution equations of plasticity and damage.

The plastic multiplier, $\dot{\lambda}_p$ can be obtained using the consistency condition for plasticity such $(\dot{f} = 0)$ that

$$\dot{f} \equiv \frac{\partial f}{\partial \sigma_{ij}} : \dot{\sigma}_{ij} + \frac{\partial f}{\partial \bar{\phi}_{ij}} : \dot{\bar{\phi}}_{ij} + \frac{\partial f}{\partial \bar{X}_{ij}} : \dot{\bar{X}}_{ij} + \frac{\partial f}{\partial \bar{R}} \dot{\bar{R}} = 0. \tag{7.20}$$

7.2. Thermodynamic potential of damage

The following form of the damage potentials for a composite is defined here:

$$G^{(u)} = g^{(u)} + \frac{k_d}{2} \bar{\Gamma}_{ij}^{(u)} \bar{\Gamma}_{ij}^{(u)}. \tag{7.21}$$

Similar to Eq. (7.12), k_d is a constant to adjust the units of the equation, and $g^{(u)}$ represents the non-local, gradient-dependent damage criterion and is defined as follows

$$g^{(u)} = \left(\bar{Y}_{ij}^{(u)} - \bar{\Gamma}_{ij}^{(u)}\right) \bar{P}_{ijkl}^{(u)} \left(\bar{Y}_{kl}^{(u)} - \bar{\Gamma}_{kl}^{(u)}\right) - 1 \leq 0. \tag{7.22}$$

The fourth order tensor $\bar{P}_{ijkl}$ describes the anisotropic nature of the damage growth and the initiation of damage. Its form is given as a function of the hardening tensor $\tilde{h}$:

$$\bar{P}_{ijkl}^{(u)} = \tilde{h}_{ij}^{(u)^{-1}} \tilde{h}_{kl}^{(u)^{-1}}, \tag{7.23}$$

$\tilde{h}_{kl}^{(u)^{-1}}$ is the inverse of the tensor $\tilde{h}^{(u)}$,

$$\tilde{h}_{ij}^{(u)} = \left(\lambda\eta\left(\frac{\bar{\kappa}^{(u)}}{\lambda}\right)^{\xi} \bar{\phi}_{ij}^{(u)} + \delta_{ij}\lambda v^2\right) \tag{7.24}$$

where ξ, η, λ, and v are material parameters related to damage [12] and the non-local damage term $\bar{\kappa}^{(u)}$ is defined by Eq. (4.16).

Using the generalized and normality rule of thermodynamics, the evolution equations can be defined for the internal state variables for damage as follows:

$$\overset{(d)}{(1)}\dot{\kappa}^{(u)} = -\dot{\lambda}_d \frac{\partial G^{(u)}}{\partial \overset{(d)}{(1)} K^{(u)}} = -\dot{\lambda}_d \overset{(d)}{(1)} \tilde{B}^{(u)} \frac{\partial g^{(u)}}{\partial \bar{K}^{(u)}}, \tag{7.25}$$

$$\overset{(d)}{(2)}\dot{\kappa}^{(u)} = -\dot{\lambda}_d \frac{\partial G^{(u)}}{\partial \overset{(d)}{(2)} K^{(u)}} = -\dot{\lambda}_d \overset{(d)}{(2)} \tilde{B}^{(u)} \frac{\partial g^{(u)}}{\partial \bar{K}^{(u)}}, \tag{7.26}$$

$$(7.27) \qquad \overset{(d)}{(3)}\dot{\kappa}^{(u)} = -\dot{\lambda}_d \frac{\partial G^{(u)}}{\partial \overset{(d)}{(3)} K^{(u)}} = -\dot{\lambda}_d \overset{(d)}{(3)}\tilde{B}^{(u)} \frac{\partial g^{(u)}}{\partial \bar{K}^{(u)}},$$

$$(7.28) \qquad \overset{(d)}{(1)}\dot{\gamma}_{ij}^{(u)} = -\dot{\lambda}_d \frac{\partial G^{(u)}}{\partial \overset{(d)}{(1)}\Gamma_{ij}^{(u)}} = -\dot{\lambda}_d \overset{(d)}{(1)}\tilde{A}^{(u)} \left\{ \frac{\partial g^{(u)}}{\partial \bar{\Gamma}_{ij}^{(u)}} + k_d \bar{\Gamma}_{ij}^{(u)} \right\},$$

$$(7.29) \qquad \overset{(d)}{(2)}\dot{\gamma}_{ij}^{(u)} = -\dot{\lambda}_d \frac{\partial G^{(u)}}{\partial \overset{(d)}{(2)}\Gamma_{ij}^{(u)}} = -\dot{\lambda}_d \overset{(d)}{(2)}\tilde{A}^{(u)} \left\{ \frac{\partial g^{(u)}}{\partial \bar{\Gamma}_{ij}^{(u)}} + k_d \bar{\Gamma}_{ij}^{(u)} \right\},$$

$$(7.30) \qquad \overset{(d)}{(3)}\dot{\gamma}_{ij}^{(u)} = -\dot{\lambda}_d \frac{\partial G^{(u)}}{\partial \overset{(d)}{(3)}\Gamma_{ij}^{(u)}} = -\dot{\lambda}_d \overset{(d)}{(3)}\tilde{A}^{(u)} \left\{ \frac{\partial g^{(u)}}{\partial \bar{\Gamma}_{ij}^{(u)}} + k_d \bar{\Gamma}_{ij}^{(u)} \right\},$$

The damage multiplier $\dot{\lambda}_d$ can be obtained using the consistency condition for damage ($\dot{g} = 0$). The damage consistency condition is given as follows:

$$(7.31) \qquad \dot{g}^{(u)} = \frac{\partial g^{(u)}}{\partial \sigma} : \dot{\sigma} + \frac{\partial g^{(u)}}{\partial \bar{Y}_{ij}^{(u)}} : \dot{\bar{Y}}_{ij}^{(u)} + \frac{\partial g^{(u)}}{\partial \bar{K}^{(u)}} \dot{\bar{K}}^{(u)} + \frac{\partial g^{(u)}}{\partial \bar{\Gamma}_{ij}^{(u)}} : \dot{\bar{\Gamma}}_{ij}^{(u)} = 0.$$

8. Computational issues of the gradient approach

In this work, for the specific examination of interfacial damage, the internal state variables are reduced as will be discussed. The remaining set of differential equations involve macroscale second order gradients of the internal state variables for both plasticity and damage, and a mesoscale second order gradient of the damage tensor. In order to solve such a higher order problem, the finite element approach is used here. Both the yield and damage conditions can be only satisfied in the weak form respectively.

8.1. Thermodynamic potential (augmented by some gradient terms)

In the formulation presented here the internal state variables are augmented as shown in Table 3. The average mesoscale gradients of kinematic and isotropic hardening in plasticity are eliminated since no analysis at the mesoscale level will be conducted for discrete dislocations. The average mesoscale gradients of kinematic and isotropic hardening in damage are discarded from the analysis

since no mesostructure will be used for the analysis of these variables. Also, only interface damage will be incorporated in this work such that $\bar{\phi}_{ij} = \bar{\phi}_{ij}^{(i)} = \phi_{ij}^{(i)} + {}^{(d)}C\widehat{\hat{\nabla}^2\hat{\phi}_{ij}^{(i)}}$ in order to simplify the formulation.

Eqs. (4.3) to (4.7) can now be written as follows:

$$\bar{\alpha}_{ij} = \alpha_{ij} + A\nabla^2\alpha_{ij}, \tag{8.1}$$

$$\bar{p} = p + A\nabla^2 p, \tag{8.2}$$

$$\bar{\gamma}_{ij} = \gamma_{ij}^{(i)} + A\nabla^2\gamma_{ij}^{(i)}, \tag{8.3}$$

$$\bar{\kappa} = \kappa^{(i)} + A\nabla^2\kappa^{(i)}, \tag{8.4}$$

$$\bar{\phi}_{ij} = \bar{\phi}_{ij}^{(i)} + C^{(i)}\widehat{\hat{\nabla}^2\hat{\phi}_{ij}^{(i)}}. \tag{8.5}$$

Table 3. Reduced internal state flux variables

		Macroscale Variables in RVE	Macroscale Gradient in RVE	Averaged Mesoscale Gradient in SRVE
Elastic Internal Variable	Elastic strain	${}^{(e)}_{(1)}\varepsilon_{ij} = \varepsilon'_{ij}$		
Plasticity Internal Flux Variables	Kinematic hardening	${}^{(p)}_{(1)}\alpha_{ij} = \alpha_{ij}$	${}^{(p)}_{(2)}\alpha_{ij} = \nabla^2\alpha_{ij}$	
	Isotropic hardening	${}^{(p)}_{(1)}p = p$	${}^{(p)}_{(2)}p = \nabla^2 p$	
Damage Internal	Damage tensor	${}^{(d)}_{(1)}\phi_{ij}^{(i)} = \phi_{ij}^{(i)}$		${}^{(d)}_{(3)}\phi_{ij}^{(i)} = \widehat{\hat{\nabla}^2\phi_{ij}^{(i)}}$
	Kinematic hardening	${}^{(d)}_{(1)}\alpha_{ij}^{(i)} = \alpha_{ij}^{(i)}$	${}^{(d)}_{(2)}\alpha_{ij}^{(i)} = \nabla^2\alpha_{ij}^{(i)}$	
	Isotropic hardening	${}^{(d)}_{(1)}\kappa^{(i)} = \kappa^{(i)}$	${}^{(d)}_{(2)}\kappa^{(i)} = \nabla^2\kappa^{(i)}$	

8.2. Discretization of the displacement field

Starting with the displacement field discretization one can write [15]:

$$\int \delta\mathbf{u}^T(\mathbf{L}^T\sigma_{j+1})dV = 0, \tag{8.6}$$

where the superscript T is the transpose symbol, denotes the variation of a term, and $\mathbf{L}$ is a differential operator given as follows:

$$\mathbf{L}^T = \begin{bmatrix} \frac{\partial}{\partial x} & 0 & 0 & \frac{\partial}{\partial y} & 0 & \frac{\partial}{\partial z} \\ 0 & \frac{\partial}{\partial y} & 0 & \frac{\partial}{\partial x} & \frac{\partial}{\partial z} & 0 \\ 0 & 0 & \frac{\partial}{\partial z} & 0 & \frac{\partial}{\partial y} & \frac{\partial}{\partial x} \end{bmatrix}. \tag{8.7}$$

σ_{j+1} contains the stress components and can be decomposed as $\sigma_j + d\sigma$ where $d\sigma$ is defined as follows [12]:

$$d\sigma = \mathbf{E}d\varepsilon' + \frac{\partial \mathbf{M}^{-1}}{\partial \bar{\phi}} \dot{\bar{\phi}} \tilde{\mathbf{E}} \varepsilon', \tag{8.8}$$

where $\mathbf{E}$ is the damaged elastic stiffness tensor and $\tilde{\mathbf{E}}$ is the undamaged elastic stiffness tensor. $\mathbf{M}$ is an overall damage effect tensor such that

$$\tilde{\sigma} = \mathbf{M}\sigma \tag{8.9}$$

where $\tilde{\sigma}$ is the undamaged stress tensor. VOYIADJIS and PARK [13] have shown that the fourth order tensor for damage $\mathbf{M}^{(u)}$ for each constituent may be expressed in terms of the second order damage tensor $\bar{\phi}^{(u)}$ where u=m,f,i. Also, VOYIADJIS and PARK [13] have shown that the total damage tensor $\mathbf{M}$ may be expressed in terms of the individual damages as:

$$\mathbf{M} = \left(\tilde{c}^{(m)} \mathbf{M}^{(m)} \tilde{\mathbf{B}}^{(m)} + \tilde{c}^{(f)} \mathbf{M}^{(f)} \tilde{\mathbf{B}}^{(f)} \right) \mathbf{M}^{(i)} \tag{8.10}$$

where $\tilde{\mathbf{B}}^{(m)}$ and $\tilde{\mathbf{B}}^{(f)}$ denote the effective undamaged configuration stress concentration tensors for the matrix and fiber, respectively, and $\tilde{c}^{(m)}$ and $\tilde{c}^{(f)}$ denote the effective undamaged configuration volume fractions for the matrix and fiber, respectively. Since we are just considering interfacial damage here, the overall damage effect tensor is given as:

$$\mathbf{M} = \left(\tilde{c}^{(m)} \mathbf{I} \tilde{\mathbf{B}}^{(m)} + \tilde{c}^{(f)} \mathbf{I} \tilde{\mathbf{B}}^{(f)} \right) \mathbf{M}^{(i)} = \mathbf{I}\mathbf{M}^{(i)} = \mathbf{M}^{(i)} \tag{8.11}$$

where $\mathbf{I}$ is the identity tensor. One can now obtain $\bar{\phi}$ from M and use $\bar{\phi}$ in Eq. (8.8) to obtain $d\sigma$.

Substitution of the evolution equations given by Eqs. (7.8) and (7.11) with the appropriate simplifications gives:

$$(8.12)\quad d\sigma = \mathbf{E}\left(d\varepsilon - \dot{\lambda}_p \frac{\partial f}{\partial \sigma}\right) - \frac{\partial \mathbf{M}^{-1}}{\partial \bar{\phi}}\left(\dot{\lambda}_p \frac{\partial f}{\partial \bar{\mathbf{Y}}^{(i)}} + \dot{\lambda}_d \frac{\partial g^{(i)}}{\partial \bar{\mathbf{Y}}^{(i)}}\right) \left(\begin{smallmatrix}(d)\\(1)\end{smallmatrix}\tilde{C}^{(i)} + \begin{smallmatrix}(d)\\(3)\end{smallmatrix}C^{(i)}\begin{smallmatrix}(d)\\(3)\end{smallmatrix}\tilde{C}^{(i)}\right)\tilde{\mathbf{E}}\varepsilon'$$

which can be written as follows:

$$(8.13)\quad d\sigma = \mathbf{E}\left(d\varepsilon - \dot{\lambda}_p \chi_p\right) - \dot{\lambda}_d \chi_d,$$

where the following tensors have been introduced:

$$(8.14)\quad \chi_p = \frac{\partial f}{\partial \sigma} + \frac{\partial \mathbf{M}^{-1}}{\partial \bar{\phi}} \frac{\partial f}{\partial \bar{\mathbf{Y}}^{(i)}} \left(\begin{smallmatrix}(d)\\(1)\end{smallmatrix}\tilde{C}^{(i)} + \begin{smallmatrix}(d)\\(3)\end{smallmatrix}C^{(i)}\begin{smallmatrix}(d)\\(3)\end{smallmatrix}\tilde{C}^{(i)}\right)\tilde{\mathbf{E}}\varepsilon',$$

$$(8.15)\quad \chi_d = \frac{\partial \mathbf{M}^{-1}}{\partial \bar{\phi}} \frac{\partial g^{(i)}}{\partial \bar{\mathbf{Y}}^{(i)}} \left(\begin{smallmatrix}(d)\\(1)\end{smallmatrix}\tilde{C}^{(i)} + \begin{smallmatrix}(d)\\(3)\end{smallmatrix}C^{(i)}\begin{smallmatrix}(d)\\(3)\end{smallmatrix}\tilde{C}^{(i)}\right)\sigma.$$

The standard boundary conditions and small deformation strains, ε are defined in the following equations [15]:

$$(8.16)\quad \Sigma \nu_s = \mathbf{t}, \qquad \mathbf{u} = \mathbf{u}_s,$$

$$(8.17)\quad \varepsilon = \mathbf{L}\mathbf{u},$$

where Σ is the stress tensor in matrix form, ν_s is the outward normal to a surface S and $\mathbf{t}$ is the boundary traction vector.

Integrating by parts and using the standard boundary conditions, Eq. (8.6) can be rewritten as follows [15]

$$(8.18)\quad \int_V \delta\varepsilon^T \, d\sigma \, dV = \int_S \delta\mathbf{u}^T \, \mathbf{t}_{j+1} \, dS - \int_V \delta\varepsilon^T \, \sigma_j dV.$$

where $\mathbf{t}_{j+1}$ are the tractions on the boundary. Using Eq. (8.13) in Eq. (8.18) one can obtain the following relation:

$$\int_V \delta\varepsilon^T \left\{ \mathbf{E}\left(d\varepsilon - \dot{\lambda}_p \chi_p\right) - \dot{\lambda}_d \chi_d \right\} dV = \int_S \delta \mathbf{u}^T \mathbf{t}_{j+1} dS - \int_V \delta\varepsilon^T \sigma_j dV. \tag{8.19}$$

The discretization procedure for the displacement field $\mathbf{u}$ requires C^0 continuous interpolation functions assembled in the shape function $\mathbf{N}$, such that

$$\mathbf{u} = \mathbf{N}\mathbf{a} \tag{8.20}$$

where $\mathbf{a}$ is the nodal displacement vector. The discretization of the strain from the linear kinematic relation is given as follows

$$\varepsilon = \mathbf{B}\mathbf{a} = \mathbf{L}\mathbf{N}\mathbf{a}, \tag{8.21}$$

where $\mathbf{B}$ is a matrix that relates the strain and the displacement.

The discretization of the multipliers, λ_p and λ_d, requires the C^1 continuous shape function contained in $\mathbf{h}$

$$\dot{\lambda}_p = \mathbf{h}^T \dot{\Lambda}_p, \qquad \dot{\lambda}_p = \mathbf{h}^T \dot{\Lambda}_d, \tag{8.22}$$

where Λ_p and Λ_d denote vectors of the nodal degrees of freedom for the plastic and damage multiplier field, respectively.

The discretization of the gradients of the multipliers will require the matrices $\mathbf{p} = \nabla\mathbf{h}$ and $\mathbf{q} = \nabla^2\mathbf{h}$ so that [15]:

$$\nabla d\lambda_p = \mathbf{p}^T d\Lambda_p, \qquad \nabla d\lambda_d = \mathbf{p}^T d\Lambda_d, \tag{8.23}$$

$$\nabla^2 d\lambda_p = \mathbf{q}^T d\Lambda_p, \qquad \nabla^2 d\lambda_d = \mathbf{q}^T d\Lambda_d. \tag{8.24}$$

Using Eqs. (8.21) and (8.22) in Eq. (8.19), the discretized equilibrium equation can be written as follows:

$$\delta\mathbf{a}^T \int_V \mathbf{B}^T \left\{ \mathbf{E}\mathbf{B}\dot{\mathbf{a}} - \mathbf{E}\chi_p \mathbf{h}^T \dot{\Lambda}_p - \chi_p \mathbf{h}^T \dot{\Lambda}_d \right\} dV = \delta\mathbf{a}^T \left\{ \int_S \mathbf{N}^T \mathbf{t}_{j+1} dS - \int_V \mathbf{B}^T \sigma_j dV \right\}. \tag{8.25}$$

8.3. Discretization of the yield condition

A second set of linear system of equations may be obtained by using the yield condition that is satisfied in a distributed sense such that

A second set of linear system of equations may be obtained by using the yield condition that is satisfied in a distributed sense such that

$$\int_V \delta\lambda_p F\left(\sigma_{j+1},\, p_{j+1},\, \nabla^2 p_{j+1},\, \alpha_{j+1},\, \nabla^2\alpha_{j+1}\right) dV = 0. \tag{8.26}$$

One can expand the yield potential, F_{j+1}, around $[\sigma_j, p_j, \nabla^2 p_j, \alpha_j, \nabla^2\alpha_j]$ by using the Taylor series in the following form:

$$F_{j+1} = F_j + \left(\frac{\partial F}{\partial \sigma}\right)_j^T d\sigma + \frac{\partial F}{\partial p}\, dp + \frac{\partial F}{\partial \nabla^2 p}\, d\nabla^2 p + \left(\frac{\partial f}{\partial \alpha}\right)_j^T d\alpha + \left(\frac{\partial F}{\partial \nabla^2 \alpha}\right)_j^T d\nabla^2\alpha. \tag{8.27}$$

The evolution equations for the isotropic and kinematic hardening terms and the corresponding gradients are given here from Eqs. (7.14)-(7.15) and (7.17)-(7.18) as

$$d\alpha = -d\lambda_p \, {}^{(p)}_{(1)}\tilde{A}\left\{\frac{\partial f}{\partial \bar{\mathbf{X}}} + k_p\, \bar{\mathbf{X}}\right\}, \qquad dp = d\lambda_p \, {}^{(p)}_{(1)}\tilde{B}. \tag{8.28}$$

$$\nabla^2 d\alpha = -d\lambda_p \, {}^{(p)}_{(2)}\tilde{A}\left\{\frac{\partial f}{\partial \bar{\mathbf{X}}} + k_p\, \bar{\mathbf{X}}\right\}, \qquad \nabla^2 dp = d\lambda_p \, {}^{(p)}_{(2)}\tilde{B}. \tag{8.29}$$

Alternatively, the evolution equations for the gradient terms can be obtained directly by operating on Eqs. (8.28) with the laplacian. Thus, the evolution equations are given as

$$d\alpha = d\lambda_p\, \eta_1^p, \tag{8.30}$$

$$\nabla^2 d\alpha = \eta_1^p \nabla^2 d\lambda_p + 2\nabla d\lambda_p \nabla\eta_1^p + d\lambda_p \nabla^2 \eta_1^p, \tag{8.31}$$

$$dp = d\lambda_p \eta_2^p, \tag{8.32}$$

$$\nabla^2 dp = \eta_2^p \nabla^2 d\lambda_p, \tag{8.33}$$

where

$$\eta_1^p = -\overset{(p)}{(1)}\tilde{A}\left\{\frac{\partial f}{\partial \bar{\bar{\mathbf{X}}}} + k_p \bar{\mathbf{X}}\right\}, \tag{8.34}$$

$$\eta_2^p = \overset{(p)}{(1)}\tilde{B}. \tag{8.35}$$

Using Eqs. (8.30) to (8.33), the discretized yield potential in Eq. (8.27) can be rewritten in terms of the plastic multiplier, $d\lambda_p$ in the following way:

$$F_{j+1} = F_j + \left(\frac{\partial F}{\partial \sigma}\right)_j^T d\sigma + \eta_2^p \left\{\left(\frac{\partial F}{\partial p}\right)_j d\lambda_p + \left(\frac{\partial F}{\partial \nabla^2 p}\right)_j \nabla^2 d\lambda_p\right\} + \left\{\left(\frac{\partial F}{\partial \alpha}\right)_j^T \eta_1^p d\lambda_p + \left(\frac{\partial F}{\partial \nabla^2 \alpha}\right)_j^T \left\{\eta_1^p \nabla^2 d\lambda_p + 2\nabla \eta_1^p \nabla d\lambda_p \nabla^2 \eta_1^p\right\}\right\}. \tag{8.36}$$

Equation (8.36) may be rewritten in terms of the plastic multiplier and its gradients such that

$$F_{j+1} = F_j + \mathbf{m}_p^T \mathbf{E} d\varepsilon + \left(n_p + \mathbf{g}_p + \mathbf{g}'_{p1} - \mathbf{m}_p^T \mathbf{E} \chi_p\right) d\lambda_p + \mathbf{g}'_{p2} \nabla d\lambda_p + \left(n'_p + \mathbf{g}'_{p3}\right) \nabla^2 d\lambda_p - \mathbf{m}_p^T \chi_d d\lambda_d, \tag{8.37}$$

where,

$$\mathbf{m}_p = \left(\frac{\partial F}{\partial \sigma}\right)_j, \tag{8.38}$$

$$n_p = \eta_2^p \left(\frac{\partial F}{\partial \sigma}\right)_j, \tag{8.39}$$

$$n'_p = \eta_2^p \left(\frac{\partial F}{\partial \nabla^2 p}\right), \tag{8.40}$$

$$\mathbf{g}_p = \left(\frac{\partial F}{\partial \alpha}\right)_j^T \eta_1^p, \tag{8.41}$$

$$\mathbf{g}'_{p1} = \left(\frac{\partial F}{\partial \nabla^2 \alpha}\right)_j^T \nabla^2 \eta_1^p, \qquad \mathbf{g}'_{p2} = 2\left(\frac{\partial F}{\partial \nabla^2 \alpha}\right)_j^T \nabla^2 \eta_1^p,$$

(8.42)

$$\mathbf{g}'_{p3} = \left(\frac{\partial F}{\partial \nabla^2 \alpha}\right)_j^T \eta_1^p.$$

Substituting Eqs. (8.21) - (8.24) and (8.37) in Eq. (8.37), one can obtain the discretized yield condition in the following form:

$$(8.43) \quad -\delta\Lambda_p^T \int_V \mathbf{h}\Big\{\Big[\Big(n_p + \mathbf{g}_p + \mathbf{g}'_{p1} - \mathbf{m}_p^T \mathbf{E}\chi_p\Big)\mathbf{h}^T + \mathbf{g}'_{p2}\mathbf{p}^T$$

$$+ \Big(n'_p + \mathbf{g}'_{p3}\Big)\mathbf{q}^T\Big] d\Lambda_p + \mathbf{m}_p^T \mathbf{E}\mathbf{B} d\mathbf{a} - \mathbf{m}_p^T \chi_d \mathbf{h}^T d\Lambda_d\Big\} dV = \delta\Lambda_p^T \int \mathbf{h} F_j dV,$$

which is valid provided that the nonstandard boundary conditions for plasticity given in the following expressions [15]:

$$(8.44) \qquad \delta\lambda_p = 0, \qquad \text{or} \qquad (\nabla d\lambda_p)\,\nu_p = 0$$

are valid on the elastic-plastic boundary S_p. The detailed explanation for the nonstandard boundary conditions of plasticity is given by [2] and [15].

8.4. Discretization of the damage condition

A third set of linear system of equations may be obtained by using the discretized damage condition

$$(8.45) \qquad \int_V \delta\lambda_d G\Big(\phi_{j+1},\ \overline{\hat{\nabla}^2 \hat{\phi}_{j+1}},\ \kappa_{j+1},\ \nabla^2\kappa_{j+1},\ \gamma_{j+1},\ \nabla^2\gamma_{j+1}\Big) dV = 0.$$

One can expand Eq. (8.45) around $[\phi_j \widehat{\hat{\nabla}^2 \hat{\phi}_j}, \kappa_j, \nabla^2\kappa_j, \gamma_j, \nabla^2\gamma_j]$ by using the Taylor series in the following way:

$$(8.46) \quad G_{j+1} = G_j + \left(\frac{\partial G}{\partial \sigma}\right)_j^T d\sigma + \left(\frac{\partial G}{\partial \phi}\right)_j^T d\phi + \left(\frac{\partial G}{\partial \overline{\hat{\nabla}^2 \hat{\phi}}}\right)_j^T d\widehat{\hat{\nabla}^2 \hat{\phi}_j}$$

$$+ \left(\frac{\partial G}{\partial \kappa}\right)_j d\kappa + \left(\frac{\partial G}{\partial \nabla^2 \kappa}\right)_j d\nabla^2\kappa + \left(\frac{\partial G}{\partial \gamma}\right)_j d\gamma + \left(\frac{\partial G}{\partial \nabla^2 \gamma}\right)_j d\nabla^2\gamma.$$

The evolution equations for the isotropic and kinematic damage hardening and the corresponding gradients are derived from Eqs. (7.28) and (7.25) in the same way as Eqs. (8.30) to (8.33) and are given as follows:

$$d\gamma = \eta_1^d \, d\lambda_d, \tag{8.47}$$

$$\nabla^2 d\gamma = \eta_1^d \nabla^2 d\lambda_d + 2\nabla d\lambda_d \nabla \eta_1^d + d\lambda_d \, \nabla^2 \eta_1^d, \tag{8.48}$$

$$d\kappa = \eta_2^d \, d\lambda_d, \tag{8.49}$$

$$\nabla^2 d\kappa = \eta_2^d \nabla^2 \, d\lambda_d, \tag{8.50}$$

where

$$\eta_1^d = -\overset{(d)}{\underset{(1)}{\tilde{A}}} \left\{ \frac{\partial g}{\partial \bar{\Gamma}} + k_d \bar{\Gamma} \right\}, \tag{8.51}$$

$$\eta_2^d = -\overset{(d)}{\underset{(1)}{\tilde{B}}} \frac{\partial g}{\partial \bar{K}}. \tag{8.52}$$

The damage tensor and the average mesoscale gradient of the damage tensor will be used in the following form from Eqs. (7.5) and(7.7):

$$d\phi = \eta_3^{dp} \, d\lambda_p + \eta_3^{dd} \, d\lambda_d, \tag{8.53}$$

$$\overline{\hat{\nabla}^2 d\hat{\phi}} = \hat{\eta}_3^{dp} d\lambda_p + \hat{\eta}_3^{dd} d\lambda_d, \tag{8.54}$$

where

$$\eta_3^{dp} = -\overset{(d)}{\underset{(1)}{\tilde{C}}} \frac{\partial f}{\partial \bar{Y}}, \qquad \eta_3^{dd} = -\overset{(d)}{\underset{(1)}{\tilde{C}}} \frac{\partial g}{\partial \bar{Y}} \tag{8.55}$$

$$\hat{\eta}_3^{dp} = -\overset{(d)}{\underset{(3)}{\tilde{C}}} \frac{\partial f}{\partial \bar{Y}}, \qquad \hat{\eta}_3^{dd} = -\overset{(d)}{\underset{(3)}{\tilde{C}}} \frac{\partial g}{\partial \bar{Y}} \tag{8.56}$$

Using Eqs. (8.47) to (8.50) and Eqs. (8.53) to (8.54), the discretized damage condition in Eq. (8.45) can be rewritten in terms of the damage multiplier, $d\lambda_d$

in the following form:

$$
\begin{aligned}
(8.57)\quad G_{j+1} = G_j &+ \left(\frac{\partial G}{\partial \phi}\right)_j^T \left(\mathbf{E}\left(d\varepsilon - d\lambda_p \chi_p\right) - d\lambda_d \chi_d\right) \\
&\left(\frac{\partial G}{\partial \phi}\right)_j^T \left(\eta_3^{dp}\, d\lambda_p + \eta_3^{dd}\, d\lambda_d\right) + \left(\frac{\partial G}{\partial \widehat{\hat{\nabla}^2 \hat{\phi}}}\right)_j^T \left(\hat{\eta}_3^{dp} d\lambda_p + \hat{\eta}_3^{dd} d\lambda_d\right) \\
&+ \left\{\left(\frac{\partial G}{\partial \kappa}\right)_j \eta_2^d d\lambda_d + \left(\frac{\partial G}{\partial \nabla^2 \kappa}\right)_j \left\{\eta_2^d \nabla^2 d\lambda_d + 2\nabla \eta_2^d \nabla d\lambda_d + d\lambda_d \nabla^2 \eta_2^d\right\}\right\} \\
&+ \left\{\left(\frac{\partial G}{\partial \gamma}\right)_j^T \eta_1^d d\lambda_d + \left(\frac{\partial G}{\partial \nabla^2 \gamma}\right)_j^T \left\{\eta_1^d \nabla^2 d\lambda_d + 2\nabla \eta_1^d \nabla d\lambda_d + d\lambda_d \nabla^2 \eta_1^d\right\}\right\}.
\end{aligned}
$$

Equation (8.57) may be reorganized in terms of the damage multiplier and its gradients such that

$$
\begin{aligned}
(8.58)\quad G_{j+1} = G_j &+ \mathbf{m}_d^T \mathbf{E} d\varepsilon + \left(-\mathbf{E}\mathbf{m}_d^T \chi_d + \mathbf{r}_{dp} + \hat{\mathbf{r}}_{dp}\right) d\lambda_p \\
&+ \left(-\mathbf{m}_d^T \chi_d + \mathbf{r}_{dd} + \hat{\mathbf{r}}_{dd} + n_d + n'_{d1} + \mathbf{g}_d + \mathbf{g}'_{d1}\right) d\lambda_d \\
&+ \left(n'_{d2} + \mathbf{g}'_{d2}\right) \nabla d\lambda_d + \left(n'_{d3} + \mathbf{g}'_{d3}\right) \nabla^2 d\lambda_d,
\end{aligned}
$$

where:

$$
(8.59)\qquad \mathbf{m}_d = \frac{\partial G}{\partial \sigma}
$$

$$
(8.60)\qquad \mathbf{r}_{dd} = \left(\frac{\partial G}{\partial \phi}\right)_j^T \eta_3^{dd}, \qquad \mathbf{r}_{dp} = \left(\frac{\partial G}{\partial \phi}\right)_j^T \eta_3^{dp},
$$

$$
(8.61)\qquad \hat{\mathbf{r}}_{dd} = \left(\frac{\partial G}{\partial \widehat{\hat{\nabla}^2 \hat{\phi}}}\right)_j^T \hat{\eta}_3^{dd}, \qquad \hat{\mathbf{r}}_{dp} = \left(\frac{\partial G}{\partial \widehat{\hat{\nabla}^2 \hat{\phi}}}\right)_j^T \hat{\eta}_3^{dp}
$$

$$
(8.62)\qquad n_d = \left(\frac{\partial G}{\partial \kappa}\right)_j \eta_2^d,
$$

$$
(8.63)\qquad n'_{d1} = \left(\frac{\partial G}{\partial \nabla^2 \kappa}\right)_j \nabla^2 \eta_2^d, \qquad n'_{d2} = 2\left(\frac{\partial G}{\partial \nabla^2 \kappa}\right)_j \nabla \eta_2^d,
$$

$$
n'_{d3} = \left(\frac{\partial G}{\partial \nabla^2 \kappa}\right)_j \eta_2^d,
$$

$$g_d = \left(\frac{\partial G}{\partial \gamma}\right)_j^T \eta_1^d, \tag{8.64}$$

$$g'_{d1} = \left(\frac{\partial G}{\partial \nabla^2 \gamma}\right)_j^T \nabla^2 \eta_1^d, \qquad g'_{d2} = 2\left(\frac{\partial G}{\partial \nabla^2 \gamma}\right)_j^T \nabla \eta_1^d,$$
$$g'_{d3} = \left(\frac{\partial G}{\partial \nabla^2 \gamma}\right)_j^T \eta_1^d. \tag{8.65}$$

Substituting Eqs. (8.21) - (8.24) and (8.58) in Eq. (8.45), the following expression is obtained:

$$\begin{aligned} \delta\Lambda_d \int_V \{ & -\mathbf{h}\mathbf{m}_d^T \mathbf{E}\mathbf{B} d\mathbf{a} + \mathbf{h}\left(-\mathbf{E}\mathbf{m}_d^T \chi_d + \mathbf{r}_{dp} + \hat{\mathbf{r}}_{dp}\right)\mathbf{h}^T d\Lambda_p \\ & + \mathbf{h}\left(-\mathbf{m}_d^T \chi_d + \mathbf{r}_{dd}\mathrm{d} + \hat{\mathbf{r}}_{dd} + n_d + n'_{d1} + \mathbf{g}_d + \mathbf{g}'_{d1}\right)\mathbf{h}^T d\Lambda_d \\ & + \left(n'_{d2} + \mathbf{g}'_{d2}\right)\mathbf{h}\mathbf{p}^T d\Lambda_d + \left(n'_{d3} + \mathbf{g}'_{d3}\right)\mathbf{h}\mathbf{q}^T d\Lambda_d \} \, dV = \delta\Lambda_d \int G_j h_d dV, \end{aligned} \tag{8.66}$$

which is valid provided that the non-standard boundary conditions for damage given in the following expression:

$$\delta\lambda_d = 0, \qquad \text{or} \qquad (\nabla d\lambda_d)\,\nu_d = 0 \tag{8.67}$$

are valid on the undamaged-damaged boundary S_d. For the undamaged material, the damage multiplier is $\lambda_d = 0$, so that at the boundary where damage starts to initiate, it must be ensured that $\nabla^2 \lambda_d > 0$. The dependence of the damage condition on the Laplacian of the damage internal state variables is essential for the crack interaction in order for damage localization to occur at the macroscale.

8.5. Combined discretization equations

Combining Eqs.(8.25), (8.43) and (8.66), one can obtain a set of algebraic equations in terms of the variations $da, d\Lambda_p$ and $d\Lambda_d$

$$\begin{bmatrix} \mathbf{K}_{aa} & \mathbf{K}_{a\lambda_p} & \mathbf{K}_{a\lambda_d} \\ \mathbf{K}_{\lambda_p a} & \mathbf{K}_{\lambda_p\lambda_p} & \mathbf{K}_{\lambda_p\lambda_d} \\ \mathbf{K}_{\lambda_d a} & \mathbf{K}_{\lambda_d\lambda_p} & \mathbf{K}_{\lambda_d\lambda_d} \end{bmatrix} \begin{bmatrix} d\mathbf{a} \\ d\Lambda_p \\ d\Lambda_d \end{bmatrix} = \begin{bmatrix} \mathbf{f}_e + f_a \\ \mathbf{f}_{\lambda_p} \\ \mathbf{f}_{\lambda_d} \end{bmatrix} \tag{8.68}$$

where the diagonal matrices are defined as follows:

$$\mathbf{K}_{aa} = \int_V \mathbf{B}^T \mathbf{E} \mathbf{B} dV, \tag{8.69}$$

$$\mathbf{K}_{\lambda_p \lambda_p} = -\int \mathbf{h} \Big[\Big(n_{\mathrm{p}} + \mathbf{g}_p + \mathbf{g}'_{p1} - \mathbf{m}_p^T \mathbf{E} \chi_p \Big) \mathbf{h}^T + \mathbf{g}'_{p2} \mathbf{p}^T + \Big(n'_{\mathrm{p}} + \mathbf{g}'_{p3} \Big) \mathbf{q}^T \Big] dV, \tag{8.70}$$

$$\mathbf{K}_{\lambda_d \lambda_d} = \int_V \mathbf{h} \Big\{ \Big(-\mathbf{m}_d^T \chi_d + \mathbf{r}_{dd} + \hat{\mathbf{r}}_{dd} + n_d + n'_{d1} + \mathbf{g}_d + \mathbf{g}'_{d1} \Big) \mathbf{h}^T + \Big(n'_{d2} + \mathbf{g}'_{d2} \Big) \mathbf{p}^T + \Big(n'_{d3} + \mathbf{g}'_{d3} \Big) \mathbf{q}^T \Big\} dV, \tag{8.71}$$

and the off-diagonal matrices are given by

$$\mathbf{K}_{a\lambda_p} = -\int_V \mathbf{B}^T \mathbf{E} \chi_p \mathbf{h}^T dV, \qquad \mathbf{K}_{a\lambda_d} = -\int_V \mathbf{B}^T \chi_p \mathbf{h}^T dV, \tag{8.72}$$

$$\mathbf{K}_{\lambda_p a} = -\int_V \mathbf{h} \mathbf{m}_p^T \mathbf{E} \mathbf{B} dV, \qquad \mathbf{K}_{\lambda_p \lambda_d} = \int \mathbf{h} \mathbf{m}_p^T \chi_d \mathbf{h}^T dV, \tag{8.73}$$

$$\begin{aligned} \mathbf{K}_{\lambda_d a} &= -\int_V \mathbf{h} \mathbf{m}_d^T \mathbf{E} \mathbf{B} dV, \\ K_{\lambda_d \lambda_p} &= \int_V \mathbf{h} \left(-\mathbf{E} \mathbf{m}_d^T \chi_d + \mathbf{r}_{\mathrm{dp}} + \hat{\mathbf{r}}_{\mathrm{dp}} \right) \mathbf{h}^T dV. \end{aligned} \tag{8.74}$$

The corresponding external force vector and the nodal force vector equivalent to internal stresses is given by

$$\mathbf{f}_e = \int_S \mathbf{N}^T \mathbf{t}_{j+1} dS, \qquad \mathbf{f}_a = -\int_V \mathbf{B}^T \sigma_j dV, \tag{8.75}$$

$$\mathbf{f}_{\lambda_p} = \int_S \mathbf{F}_j \, \mathbf{h} dV, \tag{8.76}$$

$$\mathbf{f}_{\lambda_d} = \int_S \mathbf{G}_j \mathbf{h} \mathbf{d} V. \tag{8.77}$$

9. Conclusion

A thermodynamically consistent multiscale gradient enhanced approach to coupled plasticity and damage is formulated in this paper. Thermodynamically consistent constitutive equations are derived here in order to investigate such issues as size effect on the strength of the composite, strain and damage localization effects on the macroscopic response of the composite, and statistically inhomogeneity of the evolution related damage variables associated with the RVE.

This approach is based on a non-local gradient-dependent theory of plasticity and damage over multiple scales that incorporates mesoscale internal state variables and their higher order gradients at both macro and mesoscales. The interaction of the length scales is a paramount factor in understanding and controlling the material defects such as dislocation, voids, and cracks at the mesoscale and interpret them at the macroscale. The behavior of these defects is captured not only individually, but also the interaction between them and their ability to create spatio-temporal patterns under different loading conditions.

The capability of the proposed model is to simulate properly size-dependent behavior of the materials together with localization problems as was effectively proven by DE BORST *et al.* [15] for the particular case of using gradients for the accumulated plastic strain only. Consequently, the boundary value problem of the standard continuum model will remain well-posed even in the softening regime.

The gradient-enhanced continuum results in additional partial differential equations that are satisfied in a weak form. Additional nodal degrees of freedom are introduced which leads to a modified finite element formulation. The governed equations can be linearized consistently and solved within incremental iterative Newton-Raphson solution procedure.

The computational issue of this theoretical formulation with proper explanation of the proper boundary conditions associated with the gradients and evaluation of the respective material parameters will be presented in a forthcoming paper. The detailed explanation for some of the non-standard boundary conditions of plasticity is given by DE BORST *et. al* [2] and [15].

Calibration for the different material properties in the proposed approach may be difficult, or impossible for certain cases. While the proposed framework is generalized to that of plasticity coupled with damage, one needs more studies to be performed in order to assess effectively the potential applications for this framework.

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