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ON THE THERMODYNAMICAL AND VARIATIONAL CONSISTENCY OF COHESIZE ZONE MODELS AT FINITE STRAINS

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Abstract. In the present contribution, the thermodynamical and variational consistency of cohesive zone models is critically analyzed. Starting from cohesive zone models suitable for fully reversible deformation, the restrictions imposed by the second law of thermodynamics are investigated. It will be shown that a naive modeling approach leads to a contradiction of the dissipation inequality, even if a purely elastic response is desired. Based on such findings, a thermomechanically consistent model including dissipative effects is proposed. This model is finally recast into a variationally consistent form. Within the resulting model, all state variables are naturally and jointly computed by minimizing an incrementally defined potential. The predictive capabilities of this model are demonstrated by means of selected examples.

1 INTRODUCTION

Cohesive interface models dating back to the pioneering works [1, 2, 3] represent one of the most powerful and versatile tools available for the analysis of material failure. Within such models, the stress vector acting at a crack, usually given in terms of the crack width, resist the separation of the bulk material across the crack.

While the number of different cohesive interface models in the literature is tremendous (for an overview, see [4, 5] and references cited therein), interface laws specifically designed for material failure at finite strains are still relatively rare – particularly for anisotropic solids. However, geometrically nonlinear effects and anisotropic mechanical responses do play an important role in many applications, e.g., in delamination processes, cf. [6].

Clearly, considering a geometrically exact description, the constraints imposed by the fundamental principles of constitutive modeling such as those related to the principle

of objectivity are not automatically fulfilled and thus, they require special attention. However and as shown in [7], such principles are often not carefully considered. More precisely, except for the framework presented in [7], the existing cohesive zone models described with respect to the current, i.e., deformed, configuration which account for an anisotropic mechanical response, do not fulfill all of the aforementioned physical principles. Particularly, the second law of thermodynamics is not fulfilled. In the present paper, a physically sound framework complying with these fundamentals of physics is discussed.

2 KINEMATICS

In what follows, a body Ω is considered to be separated during deformation into the two parts Ω^- and Ω^+ by means of a crack or a shear band denoted as $\partial_{\mathrm{s}}\Omega$, i.e., $\Omega = \Omega^- \cup \Omega^+ \cup \partial_{\mathrm{s}}\Omega$. The orientation of $\partial_{\mathrm{s}}\Omega$ with respect to the undeformed configuration is locally defined by its normal vector $\boldsymbol{N}$. In line with standard notation, the normal vectors are postulated as $\boldsymbol{N}^- = -\boldsymbol{N}^+ = \boldsymbol{N}$.

The motion of the sub-bodies Ω^- and Ω^+ is described by the deformation mapping $\boldsymbol{\varphi}$ which can be written as $\boldsymbol{\varphi} = \mathrm{id} + \boldsymbol{u}$ with id being the identity mapping and $\boldsymbol{u}$ being the displacement field. Denoting $\boldsymbol{u}^{\pm}$ as the displacement field in Ω^+ and Ω^- and H_{s} as the Heaviside function of $\partial_{\mathrm{s}}\Omega$, a displacement field $\boldsymbol{u}$ characterizing a crack or a shear band is discontinuous and thus, it is of the type

$$\boldsymbol{u} = \boldsymbol{u}^- + H_{\mathrm{s}} \left(\boldsymbol{u}^+ - \boldsymbol{u}^- \right). \tag{1}$$

With Eq. (1), the displacement discontinuity $[\![\boldsymbol{u}]\!]$ at $\partial_{\mathrm{s}}\Omega$ can be defined as

$$[\![\boldsymbol{u}]\!] = \boldsymbol{u}^+ - \boldsymbol{u}^- \quad \forall \boldsymbol{X} \in \partial_{\mathrm{s}}\Omega. \tag{2}$$

Since the deformation in Ω^- and that in Ω^+ are in general uncoupled, the normal vectors $\boldsymbol{n}^-$ and $\boldsymbol{n}^+$ on both sides of a crack are usually not parallel. For this reason, a fictitious intermediate configuration $\bar{\boldsymbol{x}}$ between $\boldsymbol{x}^-$ and $\boldsymbol{x}^+$ is frequently introduced as

$$\bar{\boldsymbol{x}} = (1-\alpha)\, \boldsymbol{x}^- + \alpha\, \boldsymbol{x}^+, \quad \alpha \in [0;1]. \tag{3}$$

In most cases, α is set to $\alpha = 1/2$.

3 CONSTITUTIVE MODELING

3.1 Elastic interfaces

In the most general case, the mechanical response of an elastic interface can be defined by means of a Helmholtz energy of the type

$$\Psi = \Psi([\![\boldsymbol{u}]\!], \boldsymbol{a}_1, \ldots \boldsymbol{a}_n). \tag{4}$$

Here, $\boldsymbol{a}_i$ are structural vectors describing the material's symmetry. By introducing the surface deformation gradient associated with the fictitious intermediate configuration of

a deformed crack as

$$\bar{\boldsymbol{F}} = (1-\alpha)\ \boldsymbol{F}^- + \alpha\ \boldsymbol{F}^+, \qquad \alpha \in [0;1], \tag{5}$$

Eq. (4) can be re-written as

$$\Psi = \Psi(\llbracket \boldsymbol{u} \rrbracket, \boldsymbol{F}^-, \boldsymbol{F}^+, \boldsymbol{A}_1, \dots \boldsymbol{A}_n), \quad \text{with} \quad \dot{\boldsymbol{A}}_i = \boldsymbol{0}. \tag{6}$$

Here, $\boldsymbol{A}_i$ are the vectors obtained by applying a pull-back to the spatial vectors $\boldsymbol{a}_i$. With Eq. (6), the rate of the Helmholtz energy is computed as

$$\dot{\Psi} = \frac{\partial \Psi}{\partial \llbracket \boldsymbol{u} \rrbracket} \cdot \llbracket \dot{\boldsymbol{u}} \rrbracket + \frac{\partial \Psi}{\partial \bar{\boldsymbol{F}}} : \left[(1-\alpha)\ \dot{\boldsymbol{F}}^- + \alpha\ \dot{\boldsymbol{F}}^+ \right]. \tag{7}$$

It bears emphasis that the deformation gradients $\boldsymbol{F}^{\pm}$ and the displacement discontinuity $\llbracket \boldsymbol{u} \rrbracket$ are only weakly coupled ($\boldsymbol{F}^+ = \boldsymbol{F}^- + \mathrm{GRAD}\, \llbracket \boldsymbol{u} \rrbracket$)). Hence, the stress power consists of three terms in general. By introducing two stress tensors $\boldsymbol{P}^{\pm}$ of first Piola-Kirchhoff type being conjugate to the deformation gradients $\boldsymbol{F}^{\pm}$, the stress power can thus be written as

$$\overset{o}{w} = \boldsymbol{T} \cdot \llbracket \dot{\boldsymbol{u}} \rrbracket + \boldsymbol{P}^- : \dot{\boldsymbol{F}}^- + \boldsymbol{P}^+ : \dot{\boldsymbol{F}}^+. \tag{8}$$

Consequently, by applying the standard Coleman & Noll procedure, cf. [8], the constitutive equations

$$\boldsymbol{T} = \frac{\partial \Psi}{\partial \llbracket \boldsymbol{u} \rrbracket}, \quad \boldsymbol{P}^- = \frac{\partial \Psi}{\partial \boldsymbol{F}^-} = (1-\alpha)\ \frac{\partial \Psi}{\partial \bar{\boldsymbol{F}}}, \quad \boldsymbol{P}^+ = \frac{\partial \Psi}{\partial \boldsymbol{F}^+} = \alpha\ \frac{\partial \Psi}{\partial \bar{\boldsymbol{F}}} \tag{9}$$

are derived. As a result, two boundary-like laws are also implicitly defined by the Helmholtz energy (6) in addition to the classical constitutive model $(9)_1$, see also [9]. These additional tensors are required for thermomechanical consistency. This can be seen more explicitly by ignoring them. In this case, the dissipation reads

$$\mathcal{D} = \boldsymbol{T} \cdot \llbracket \dot{\boldsymbol{u}} \rrbracket - \dot{\Psi} = -\frac{\partial \Psi}{\partial \bar{\boldsymbol{F}}} : \left[(1-\alpha)\ \dot{\boldsymbol{F}}^- + \alpha\ \dot{\boldsymbol{F}}^+ \right] \neq 0. \tag{10}$$

Consequently, the dissipation would be non-vanishing, even in case of a hyperelastic-type model. It bears emphasis that these additional stress tensors have not been considered in any of the existing cohesive zone models.

3.2 Dissipative effects

In this section, the hyperelastic model described before is combined with damage mechanics. For that purpose, a Helmholtz energy of the type

$$\Psi = \sum_{i=1}^{n} \prod_{j=1}^{n} (1 - d_i^{(j)})\ \Psi_i(\llbracket \boldsymbol{u} \rrbracket, \boldsymbol{F}^+, \boldsymbol{F}^-) \tag{11}$$

is adopted. Here, $d_i^{(j)} \in [0;1]$ are damage variables. The underlying idea corresponding to Eq. (11) is that the energy is decomposed into that related to the different relevant failure modes. One typical example is given by the decomposition of the energy into mode-I and mode-II/III failure energies. Application of the Coleman & Noll procedure to Eq. (11) yields the stress response

$$\begin{aligned} \boldsymbol{T} &= \sum_{i=1}^{n} \prod_{j=1}^{n} (1 - d_i^{(j)}) \, \frac{\partial \Psi_i}{\partial [\![\boldsymbol{u}]\!]} \qquad & \boldsymbol{P}^- &= (1-\alpha) \sum_{i=1}^{n} \prod_{j=1}^{n} (1 - d_i^{(j)}) \, \frac{\partial \Psi_i}{\partial \bar{\boldsymbol{F}}} \\ & & \boldsymbol{P}^+ &= \alpha \sum_{i=1}^{n} \prod_{j=1}^{n} (1 - d_i^{(j)}) \, \frac{\partial \Psi_i}{\partial \bar{\boldsymbol{F}}}, \end{aligned} \tag{12}$$

together with the reduced dissipation inequality

$$\mathcal{D} = \mathring{w} - \dot{\Psi} = \sum_{i=1}^{n} \sum_{j=1}^{n} \prod_{k=1, k\neq j}^{n} (1 - d_i^{(k)}) \, \Psi_i([\![\boldsymbol{u}]\!], \boldsymbol{F}^+, \boldsymbol{F}^-) \, \dot{d}_i^{(j)} \geq 0. \tag{13}$$

Since the elastic energies Ψ_i are assumed to be non-negative and $d_i^{(j)} \in [0;1]$, the second law of thermodynamics is automatically fulfilled, if $d_i^{(j)}$ is monotonically increasing, i.e.,

$$\dot{d}_i^{(j)} \geq 0. \tag{14}$$

For fulfilling Ineq. (14) and also for accounting for cross-softening, the damage evolution is defined as

$$d_i^{(j)} = d_i^{(j)}(\kappa_j). \tag{15}$$

with

$$\kappa_i(t_{n+1}) = \max\{\kappa_i(t_n); \Psi_i(t_{n+1})\}, \qquad \kappa_i(t=0) = \kappa_{i(0)}. \tag{16}$$

Accordingly, κ_i is the history of the maximum stored elastic energy related to failure mode i and thus, it is monotonically increasing. Hence, if $d_i^{(j)}(\kappa_j)$ is also chosen as a monotonically increasing function, the second law of thermodynamics is automatically fulfilled. The term cross-softening results from Eq. (15) and means that mode-I crack opening leads to a reduction in the shear stiffness as well.

4 VARIATIONAL CONSTITUTIVE UPDATES

Following [7], the variational principle

$$\inf I_{\text{inc}}^{\partial_{\text{s}}\Omega}, \quad I_{\text{inc}}^{\partial_{\text{s}}\Omega} := \int_{t_n}^{t_{n+1}} \mathcal{E} \, \mathrm{d}t = \Psi(t_{n+1}) - \Psi(t_n) + \int_{t_n}^{t_{n+1}} \mathcal{D} \, \mathrm{d}t. \tag{17}$$

is equivalent to the proposed constitutive modeling framework. Thus, all state variables follow naturally from energy minimization. More explicitly,

$$(\kappa_1(t_{n+1}),\dots,\kappa_n(t_{n+1})) = \arg\inf I_{\text{inc}}^{\partial_{\text{s}}\Omega}(\llbracket \boldsymbol{u} \rrbracket_{n+1}, \bar{\boldsymbol{F}}_{n+1}, \kappa_1(t_{n+1}),\dots,\kappa_n(t_{n+1}))\big|_{\boldsymbol{u}=\text{const}}. \tag{18}$$

Finally, the reduced potential as implicitly introduced by Eq. (18) defines the stress response in the hyperelastic-like manner

$$\boldsymbol{T} = \frac{\partial \tilde{I}_{\text{inc}}^{\partial_{\text{s}}\Omega}}{\partial \llbracket \boldsymbol{u} \rrbracket}, \quad \boldsymbol{P}^{\pm} = \frac{\partial \tilde{I}_{\text{inc}}^{\partial_{\text{s}}\Omega}}{\partial \boldsymbol{F}^{\pm}}, \quad \text{with} \quad \tilde{I}_{\text{inc}}^{\partial_{\text{s}}\Omega} = \inf_{\{\kappa_i\}} I_{\text{inc}}^{\partial_{\text{s}}\Omega}. \tag{19}$$

With these notations, the total energy (work) of the considered structure is given by

$$I_{\text{total}} = I_{\text{total}}(\boldsymbol{\varphi}) = \int_{\Omega} \tilde{I}_{\text{inc}}^{\Omega}\, \mathrm{d}V - I_{\text{ext}} + \int_{\partial_{\text{s}}\Omega} \tilde{I}_{\text{inc}}^{\partial_{\text{s}}\Omega}\, \mathrm{d}A \tag{20}$$

where the potential I_{ext} is associated with external forces, while the potential $\tilde{I}_{\text{inc}}^{\Omega}$ is the bulk's counterpart of the interface-related potential $\tilde{I}_{\text{inc}}^{\partial_{\text{s}}\Omega}$. As straightforward computations shows that a minimization of potential (20) results in the classical equilibrium conditions in weak form, i.e.,

$$\delta I_{\text{total}} = 0 = \int_{\Omega} \boldsymbol{P} : \delta \boldsymbol{F}\, \mathrm{d}V - \frac{\partial I_{\text{ext}}}{\partial \boldsymbol{\varphi}} \cdot \delta \boldsymbol{u} + \int_{\partial_{\text{s}}\Omega} \left[\boldsymbol{T} \cdot \delta \llbracket \boldsymbol{u} \rrbracket + \boldsymbol{P}^{\pm} : \delta \boldsymbol{F}^{\pm} \right] \mathrm{d}A, \ \forall \delta \boldsymbol{u} \tag{21}$$

Here, Eqs. (12), together with $\boldsymbol{P} := \partial_{\boldsymbol{F}} \tilde{I}_{\text{inc}}^{\Omega}$, has been inserted. The term $\partial I_{\text{ext}}/\partial \boldsymbol{\varphi}$ is a generalized force. Eq. (21) can be conveniently discretrized by finite elements. Further details are omitted here. They can be found in [7] and will be discussed in the respective presentation.

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