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Potential-based constitutive models for cohesive interfaces: Theory, implementation and examples

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ABSTRACT

Cohesive interfaces appear in many materials or structures, e.g. composites or adhesive bonds. Originally introduced to model crack tips in fracture mechanics, cohesive zone models are used to describe the constitutive behavior of cohesive interfaces since the early 1990s. In the present contribution, the concept of generalized standard materials (GSM) is transferred from the modeling of bulk behavior to cohesive zones. The potential-based framework obtained hereby is referred to as standard dissipative cohesive zones (SD-CZ). Within this framework, an irreversible interface model is developed for the one-dimensional case and subsequently extended to three-dimensional transverse isotropy. While the potential structure of the constitutive law may be required for certain applications, it also brings benefits with regard to the numerical implementation. To the best knowledge of the authors, this is the first approach to interface modeling in a GSM-like framework, where dissipative effects like damage and softening are considered as well as normal-tangential coupling for mixed-mode decohesion. Comparisons to experimental data and existing cohesive zone models outline the capabilities of the approach.

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1. Introduction

Potential-based material modeling of solids originated mainly from the French mechanics community (e.g., [1,2]). A commonly accepted and well-established class of constitutive models is referred to as so-called generalized standard materials (GSM), also known as standard dissipative solids. They provide a powerful tool for several reasons. In the GSM framework, the constitutive behavior of the material is defined by two scalar-valued functions: the Helmholtz free energy density and the dissipation potential. This potential structure allows for a systematic analysis of the thermodynamic admissibility of the constitutive model, e.g., in the sense of nonnegative inelastic dissipation. The energy-related formulation also provides a direct link to chemo- or thermo-mechanical coupling [3,4]. Further, the structure of the constitutive equations is well-suited for an efficient numerical implementation using incremental variational formulations. Such methods have been established in the past two decades with great success (e.g., [5,6,3]). Recently, mixed variational methods considering variations of the internal variables and, simultaneously, of their conjugate forces have been proposed (e.g., [7]). They replace the dissipation

potential by its Legendre-Fenchel transform defined in the space of thermodynamic forces. Lately, the authors established a reduced basis nonlinear homogenization method relying on the potential structure of GSM in a mixed incremental variational setting [8]. In the multi-scale context, the possibility to average the potentials over reference volume elements in order to derive effective constitutive models is an important feature. Thereby, the potential structure of the microscopic constitutive model can be preserved under a change of scale which has important implications for nonlinear homogenization techniques (e.g., [9,8]).

It is long recognized that the GSM framework has its limitations, e.g. when it comes to nonlinear kinematic hardening.¹ However, many relevant material models can be reformulated in the GSM framework. Otherwise, an approximative GSM model can often substitute a non-GSM model without introducing large errors. A possible approximation of a material model in the GSM framework was for example used by Ortiz and Stainier [5] in the context of crystal plasticity with latent hardening. The hardening law that they investigated cannot be derived from a potential. Therefore, Ortiz and Stainier [5] approximated the hardening potential using a quadratic function that was adjusted in each time increment. The resulting

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¹ Models considering the nonlinear Bauschinger effect are often based on the Armstrong-Frederick model [10] and its popular extension by Chaboche [11].

incrementally defined potential structure did not introduce noticeable errors in the simulations.

While the GSM framework and the variational methods for the solution of the time-evolution problem are well-established and frequently used for bulk materials, the potential-based modeling concept with internal variables describing dissipative processes has only rarely been adapted to cohesive interface models, which are also referred to as cohesive zone models (CZM). Cohesive zone models have been first introduced in the context of cracks and slits [12,13] but are also used to describe, e.g., the interfacial behavior of adhesive bonds and polycrystalline or fiber reinforced materials [14]. Further engineering applications involving CZMs are found in electronics and micro-electro-mechanical systems (MEMS) [15]. A whole class of rather popular CZM goes back to the early proposals of Needleman [16] and Xu and Needleman [17]. They rely on a single potential for the free energy, which is often highly nonlinear. Note that these models do not contain any dissipation or path-dependency of the constitutive response with respect to the applied loading, i.e. they can be interpreted as nonlinear hyperelastic constitutive models where the traction vector depends only on the current interface opening vector. Therefore, deficiencies such as increasing forces on decreasing load can appear. In contrast to this, dissipative effects are captured in numerous recent interface models, e.g. in the works of Valoroso and Champaney [18], Musto and Alfano [19], Ottosen and Ristinmaa [20]. A Helmholtz free energy density function is involved in most of these models, but, other than in the GSM framework, dissipation is not controlled by a potential.

In the present contribution, the potential-based ansatz of GSM type is adopted for interface models in the spirit of Constanzo and Allen [21]. Dissipative processes at the interface are modeled using the internal variable concept [22]. The theoretical background is revised and a general formulation of a framework referred to as *standard dissipative cohesive zones* (SD-CZ) is given in Section 2. A specific dissipative cohesive zone model incorporating elastic degradation of the interface is developed in Section 3. The proposed model aims at the description of brittle interface behavior but could also be used to describe rate effects and pseudo-ductile failure. A key feature of this specific SD-CZM is the coupling of the dissipative processes in normal and tangential direction. Thereby, mutual coupling of the normal and tangential behavior of the interface can be accounted for. This allows for the accurate investigation of mixed-mode decohesion.

Aspects of the numerical implementation for the GSM-like class of constitutive interface models are addressed in Section 4. A mixed incremental formulation is presented. It allows for an efficient time integration procedure, and the developed structure leads to a straight-forward computational realization. The algorithmic stiffness operator is explicitly derived in the general SD-CZ framework and its unconditional symmetry is shown.

Numerical examples of the potential-based damage model from Section 3 are presented in Section 5. It is shown that the model can replicate the cohesive behavior found in experiments by Sørensen and Jacobsen [23]. Further, the model is compared to the improved Xu and Needleman cohesive zone law for mixed-mode decohesion proposed by van den Bosch et al. [24]. It has also been incorporated into a finite element model of the miniature mixed-mode bending test of Kolluri et al. [25], and the FE results are compared to experimental data of the bending test. The paper closes with a brief summary and an outlook for future applications in Section 6.

2. Potential-based constitutive modeling

2.1. Generalized standard materials

The term *generalized standard materials* (GSM) denotes a class of constitutive models for solid materials that are entirely

characterized by two scalar functions, namely the Helmholtz free energy density ψ_Ω and the dissipation potential ϕ_Ω . At this, the free energy is defined as a function of the current material state. Attention is confined to isothermal processes in the present contribution. In a geometrically linear setting, the material state is then described by the infinitesimal strain tensor $\boldsymbol{\varepsilon}$ and, possibly, a set of internal state variables $\mathcal{I}$. Following Coleman and Gurtin [22], internal variables are used to model dissipative, path-dependent material behavior.² The free energy then defines the Cauchy stress tensor $\boldsymbol{\sigma}$ and the thermodynamic driving forces $\mathcal{F}$ by

$$\boldsymbol{\sigma} = \frac{\partial \psi_\Omega(\boldsymbol{\varepsilon}, \mathcal{I})}{\partial \boldsymbol{\varepsilon}}, \quad \mathcal{F} = -\frac{\partial \psi_\Omega(\boldsymbol{\varepsilon}, \mathcal{I})}{\partial \mathcal{I}}. \quad (1)$$

The generalized forces $\mathcal{F}$ are (up to their sign) power conjugate to the rate of the internal state. They describe the resistance of the material to changes of the material state. While any purely elastic process leaves the internal variables untouched, their values are changed during an irreversible process. Hence, an evolution law for the internal variables is needed for the description of dissipative processes. In the GSM framework, such a law is defined by the dissipation potential ϕ_Ω via

$$\dot{\mathcal{I}} = \frac{\partial \phi_\Omega(\dot{\mathcal{I}})}{\partial \dot{\mathcal{I}}}. \quad (2)$$

Note that this implicit relation together with (1) defines the Biot-type equation

$$\frac{\partial \phi_\Omega(\dot{\mathcal{I}})}{\partial \dot{\mathcal{I}}} + \frac{\partial \psi_\Omega(\boldsymbol{\varepsilon}, \mathcal{I})}{\partial \mathcal{I}} = 0, \quad (3)$$

which formally defines the evolution of the internal state variables $\mathcal{I}$.

An alternative description of the evolution of the internal state in terms of the thermodynamic driving forces $\mathcal{F}$ is often favorable, either from a modeling perspective or due to numerical reasons. Such a description can be obtained from the dual dissipation potential ϕ_Ω^* which is given by the Legendre-Fenchel transform of the dissipation potential ϕ_Ω

$$\phi_\Omega^*(\mathcal{F}) = \sup_{\dot{\mathcal{I}}} \{ \mathcal{F} \cdot \dot{\mathcal{I}} - \phi_\Omega(\dot{\mathcal{I}}) \}. \quad (4)$$

It shall be noted that the dual of ϕ_Ω^* gives, again, the dissipation potential

$$\phi_\Omega(\dot{\mathcal{I}}) = \phi_\Omega^{**}(\dot{\mathcal{I}}) = \sup_{\mathcal{F}} \{ \mathcal{F} \cdot \dot{\mathcal{I}} - \phi_\Omega^*(\mathcal{F}) \}. \quad (5)$$

The gradient of the dual dissipation potential explicitly defines the rates of the internal variables via

$$\dot{\mathcal{I}} = \frac{\partial \phi_\Omega^*(\mathcal{F})}{\partial \mathcal{F}}, \quad (6)$$

assuming a differentiable dual dissipation ϕ_Ω^* . Note that the two expression (3) and (6) can both be used to model the inelastic processes in the bulk material. However, for many materials only either the primal dissipation potential ϕ_Ω or its dual ϕ_Ω^* is available. If both potentials are at hand, then the dual potential leading to the explicit evolution law (6) is usually preferred over the implicit relation defined by the Biot-type Eq. (3).

2.2. Standard dissipative cohesive zones (SD-CZ)

The GSM concept for bulk materials is now adapted to allow for a potential-based modeling of the constitutive behavior of cohesive interfaces. Following the alternative term *standard dissipative solids* for GSM, we refer to the framework for cohesive interfaces as

² Prominent examples of internal state variables are the infinitesimal plastic strain tensor, the accumulated plastic strain, or damage variables.

standard dissipative cohesive zones (SD-CZ). When considering cohesive interfaces instead of bulk material, the kinematic variable is the jump of the displacement field $\mathbf{u}(\mathbf{x})$ across the singular surface S with unit normal $\mathbf{n}$ (see also Fig. 1)

$$\delta(\mathbf{x}) = \mathbf{u}_+(\mathbf{x}) - \mathbf{u}_-(\mathbf{x}). \quad (7)$$

The part δ_t of the displacement jump δ that is parallel to the surface is given by

$$\delta_t = (\mathbf{I} - \mathbf{n} \otimes \mathbf{n})\delta = \delta_t \mathbf{m}, \quad \delta_t = \|\delta_t\|, \quad \mathbf{m} = \frac{\delta_t}{\|\delta_t\|}. \quad (8)$$

Together with the normal displacement $\delta_n = \delta \cdot \mathbf{n}$, the displacement jump, also referred to as separation, can be expressed by

$$\delta = \delta_n \mathbf{n} + \delta_t \mathbf{m}. \quad (9)$$

As a supplement to δ , a generalized vector $\hat{\mathbf{y}}$ of internal variables is introduced to describe the current state of the interface. The free surface energy density of the interface is denoted by $\psi_{\mathcal{S}}(\delta, \hat{\mathbf{y}})$. Similar to the bulk material, the free energy defines the traction vector $\mathbf{t}$ on the interface and a vector $\hat{\mathbf{z}}$ of thermodynamic driving forces for the internal variables associated with the interface $\mathcal{S}$ via

$$\mathbf{t} = \frac{\partial \psi_{\mathcal{S}}(\delta, \hat{\mathbf{y}})}{\partial \delta}, \quad \hat{\mathbf{z}} = -\frac{\partial \psi_{\mathcal{S}}(\delta, \hat{\mathbf{y}})}{\partial \hat{\mathbf{y}}}. \quad (10)$$

In analogy to the GSM models for bulk materials, a dual dissipation potential $\phi_{\mathcal{S}}^*$ is introduced. The potential $\phi_{\mathcal{S}}^*$ depends only on the vector of driving forces $\hat{\mathbf{z}}$. It defines the rates of the internal state variables due to dissipative processes via

$$\dot{\hat{\mathbf{y}}} = \frac{\partial \phi_{\mathcal{S}}^*(\hat{\mathbf{z}})}{\partial \hat{\mathbf{z}}}. \quad (11)$$

The potential $\phi_{\mathcal{S}}^*$ has to be convex in $\hat{\mathbf{z}}$.

2.2.1. Work of separation and thermodynamic consistency

In the following, the time interval $[0, T]$ is considered, and it is presupposed that the interface is undamaged and closed (i.e. $\delta = \mathbf{0}$) in the beginning. It is assumed that $\psi_{\mathcal{S}}$ can be split into an elastic part $\psi_{\mathcal{S}}^e$ which vanishes for $\delta = \mathbf{0}$ and a softening potential $\psi_{\mathcal{S}}^s$ according to

$$\psi_{\mathcal{S}}(\delta, \hat{\mathbf{y}}) = \psi_{\mathcal{S}}^e(\delta, \hat{\mathbf{y}}_e) + \psi_{\mathcal{S}}^s(\hat{\mathbf{y}}_s), \quad (12)$$

where the internal variables have been partitioned according to $\hat{\mathbf{y}} = (\hat{\mathbf{y}}_e, \hat{\mathbf{y}}_s)$. Both components of $\psi_{\mathcal{S}}$ are assumed to be nonnegative,

and it is presumed that the softening potential is zero for an undamaged interface, such that

$$\psi_{\mathcal{S}}^s(t=0) = 0 \Rightarrow \psi_{\mathcal{S}}(t=0) = 0 \quad (13)$$

holds in particular. The work of separation at time T is defined as

$$W_{\text{sep}} = \int_0^T \mathbf{t} \cdot \dot{\delta} dt. \quad (14)$$

Exploiting Eq. (10), the rate of the free energy is derived as

$$\dot{\psi}_{\mathcal{S}} = \mathbf{t} \cdot \dot{\delta} - \hat{\mathbf{z}}_e \cdot \dot{\hat{\mathbf{y}}}_e - \hat{\mathbf{z}}_s \cdot \dot{\hat{\mathbf{y}}}_s, \quad (15)$$

where $\hat{\mathbf{z}}_e$ and $\hat{\mathbf{z}}_s$ are the conjugate forces to $\hat{\mathbf{y}}_e$ and $\hat{\mathbf{y}}_s$, respectively. This result yields

$$\begin{aligned} W_{\text{sep}} &= \psi_{\mathcal{S}}(t=T) - \psi_{\mathcal{S}}(t=0) + \int_0^T \hat{\mathbf{z}}_e \cdot \dot{\hat{\mathbf{y}}}_e dt + \int_0^T \hat{\mathbf{z}}_s \cdot \dot{\hat{\mathbf{y}}}_s dt \\ &= \psi_{\mathcal{S}}^e(t=T) + \int_0^T \hat{\mathbf{z}}_e \cdot \dot{\hat{\mathbf{y}}}_e dt. \end{aligned} \quad (16)$$

Thus, the work of separation can be decomposed into the elastic part $W_e = \psi_{\mathcal{S}}^e$ and the dissipative part $W_d = \int_0^T \hat{\mathbf{z}}_e \cdot \dot{\hat{\mathbf{y}}}_e dt$. An illustration of this decomposition for the one-dimensional case discussed in Section 3.1 is given in Fig. 2. In order to assure thermodynamic consistency in an isothermal setting, the mechanical dissipation on the interface $\mathcal{D}_{\mathcal{S}}$ is required to be nonnegative

$$\mathcal{D}_{\mathcal{S}} = \hat{\mathbf{z}}_e \cdot \dot{\hat{\mathbf{y}}}_e \geq 0, \quad (17)$$

which has to hold independently of the current interface state. The thermodynamic constraint (17) is the analogon to the reduced Clausius Duhem inequality for bulk materials (see, e.g., [22]).

2.3. Comparison of SD-CZ to GSM

As outlined before, the SD-CZ framework is derived from the GSM structure. In order to better understand the massive similarity between the two approaches, we define the general kinematic variable $\mathbf{k}$ and the general internal state variables $\mathbf{y}$. Then the free energy in both frameworks has the structure

$$\psi \equiv \psi(\mathbf{k}, \mathbf{y}), \quad (18)$$

where $(\mathbf{k}, \mathbf{y})$ correspond to $(\epsilon, \mathcal{I})$ for the bulk and to $(\delta, \hat{\mathbf{y}})$ for the cohesive interface. Particularly, the free energy for both, the bulk and the interface, depends only on a kinematic variable and the internal state variables. Similarly, the thermodynamic driving forces

Fig. 1. Kinematic and static variables in the cohesive zone; undeformed state (left) and deformed state (right).

Fig. 2. An exemplary traction-separation curve with the corresponding work of separation and its elastic and dissipative parts. (Elastic unloading to the origin, as specified in Section 3.1 and depicted in Fig. 3(c), is assumed here.)

Table 1

Comparison of the GSM and the SD-CZ framework (M – mass; L – length; T – time).

		GSM (bulk)		SD-CZ (interface)	
			Dimension		Dimension
Free energy density	ψ	$\psi_\Omega(\mathbf{e}, \mathcal{I})$	$\text{ML}^{-1}\text{T}^{-2}$	$\psi_{\mathcal{S}}(\delta, \hat{\mathbf{y}})$	MT^{-2}
Kinematic variable	$\mathbf{k}$	$\mathbf{e}$	—	δ	L
Static variable	$\mathbf{s}$	$\boldsymbol{\sigma} = \partial_{\mathbf{e}}\psi_\Omega(\mathbf{e}, \mathcal{I})$	$\text{ML}^{-1}\text{T}^{-2}$	$\mathbf{t} = \partial_\delta\psi_{\mathcal{S}}(\delta, \hat{\mathbf{y}})$	$\text{ML}^{-1}\text{T}^{-2}$
Internal variables	$\mathbf{y}$	$\mathcal{I}$	Various	$\hat{\mathbf{y}}$	Various
Driving forces	$\mathbf{z}$	$\mathcal{F} = -\partial_{\mathcal{I}}\psi_\Omega(\mathbf{e}, \mathcal{I})$	Various	$\hat{\mathbf{z}} = -\partial_{\hat{\mathbf{y}}}\psi_{\mathcal{S}}(\delta, \hat{\mathbf{y}})$	Various
Dual dissipation	ϕ^*	$\phi_\Omega^*(\mathcal{F})$	$\text{ML}^{-1}\text{T}^{-3}$	$\phi_{\mathcal{S}}^*(\hat{\mathbf{z}})$	MT^{-3}
Evolution law	$\dot{\mathbf{y}}$	$\dot{\mathcal{I}} = \partial_{\mathcal{F}}\phi_\Omega^*(\mathcal{F})$	Various	$\dot{\hat{\mathbf{y}}} = \partial_{\hat{\mathbf{z}}}\phi_{\mathcal{S}}^*(\hat{\mathbf{z}})$	Various

Fig. 3. Basic properties of a damage model (see also [R1]–[R6]).

$\mathbf{z}$, the dual dissipation ϕ^* and the rate of the internal state variables are given by

$$\mathbf{z} = -\frac{\partial\psi}{\partial\mathbf{y}}, \quad \phi^* \equiv \phi^*(\mathbf{z}), \quad \dot{\mathbf{y}} = \frac{\partial\phi^*}{\partial\mathbf{z}}. \quad (19)$$

Here $\mathbf{z}$ corresponds to $\mathcal{F}$ in the bulk material and to $\hat{\mathbf{z}}$ on the interface. Similarly, the static variable

$$\mathbf{s} = \frac{\partial\psi}{\partial\mathbf{k}} \quad (20)$$

defines the stress tensor $\boldsymbol{\sigma}$ in the bulk and the traction vector $\mathbf{t}$ on the interface. The conceptual similarity of the two frameworks is also emphasized by the juxtaposition given in Table 1.

3. Damage model for cohesive interfaces

3.1. One-dimensional model

First, only cohesive behavior in the direction normal to the interface, corresponding to the properties of mode I failure, is taken into account. Some intrinsic properties of a damage model are explored for this, mathematically speaking, one-dimensional case. Based on physical considerations and numerical demands, the following requirements are imposed on the constitutive model:

- [R1] viscous behavior of overstress type is asserted³;
- [R2] a structure fitting into the potential-based framework presented in Section 2.2 is anticipated;
- [R3] a description of complete separation must be possible; by complete separation it is understood that no positive traction t_n can be transferred across the interface (Fig. 3(a));
- [R4] unless the cohesive force t_n exceeds the state-dependent critical stress $\tau_n^c \geq 0$, linear elastic behavior is asserted (Fig. 3(b));
- [R5] upon unloading, the tractions should decay linearly to zero with the interface opening δ_n (Fig. 3(c));
- [R6] for overclosure, corresponding to a negative interface open-

ing δ_n , the interface behavior is assumed to be linear elastic with constant stiffness k_n^- (Fig. 3(d)).

A model satisfying the requirements [R1]–[R6] has been identified. The proposed model, hereafter referred to as *damage SD-CZM*, considers a degradation of the elastic material properties with the possibility of a ductile transition from elastic to inelastic, i.e. damaging, behavior. Dissipative effects are accounted for via an internal variable y_1 associated with the elastic degradation and an additional state variable y_2 which is used to model the critical damage stress τ_n^c on the interface. Both components of the vector of internal state variables $\hat{\mathbf{y}}$ are defined such that they are zero in the beginning (i.e. for an undamaged interface). Their rates are assumed to be nonnegative. In accordance with the additive split (12), the Helmholtz free energy density on the interface is chosen as

$$\psi_{\mathcal{S}}(\delta_n, \hat{\mathbf{y}}) = \psi_{\mathcal{S}}^e(\delta_n, y_1) + \psi_{\mathcal{S}}^s(y_2). \quad (21)$$

The variable y_2 accounts for irreversible changes of the microstructure of the interface such as the formation of new free surfaces (e.g., microcracks). For solid materials, an equivalent internal variable is the accumulated plastic strain, which is often used to model the formation of dislocation structures leading to hardening effects. For the proposed SD-CZM, the softening potential $\psi_{\mathcal{S}}^s(y_2)$ contains the energy that was expended for the microstructural changes of the interface in the absence of elastic deformation.

The elastic part of the Helmholtz free energy density is defined by

$$\psi_{\mathcal{S}}^e(\delta_n, y_1) = \frac{1}{2} \frac{k_n^+}{1+y_1} \langle \delta_n \rangle_+^2 + \frac{1}{2} k_n^- \langle \delta_n \rangle_-^2 \quad (22)$$

such that, following the formal definition (10), the conjugate forces

$$\begin{aligned} t_n &= \frac{\partial\psi_{\mathcal{S}}^e}{\partial\delta_n} = \frac{k_n^+}{1+y_1} \langle \delta_n \rangle_+ + k_n^- \langle \delta_n \rangle_-, \\ z_1 &= -\frac{\partial\psi_{\mathcal{S}}^e}{\partial y_1} = \frac{1}{2} \frac{k_n^+}{(1+y_1)^2} \langle \delta_n \rangle_+^2 \end{aligned} \quad (23)$$

are obtained. Here, the symbols $\langle \bullet \rangle_+$ and $\langle \bullet \rangle_-$ are defined by $\langle x \rangle_{\pm} = \frac{x \pm |x|}{2}$. The parameter k_n^+ characterizes the elastic stiffness of the undamaged interface for positive values of δ_n in the absence

³ The rate-independent case can be recovered as a limit case of the constitutive model with viscous regularization.

Table 2

Physical dimensions of the model parameters and of the internal variables (M – mass; L – length; T – time).

Internal variables		Model parameters								
		Stiffnesses		Softening type A			Softening type B		Parameters of $\phi_{\mathcal{S}}^*$	
y_1	y_2	k_n^+, k_n^-	τ_0	c	m	τ_0, τ_1	c_1, c_2	τ_n^s, φ_0	$\dot{d}_0$	p
–	L	$ML^{-2}T^{-2}$	$ML^{-1}T^{-2}$	L^{-1}	–	$ML^{-1}T^{-2}$	L^{-1}	$ML^{-1}T^{-2}$	LT^{-1}	–

of inelastic processes, while k_n^- denotes the elastic stiffness for $\delta_n \leq 0$ and can be understood as a penalty parameter preventing overclosure. Notice that (22) corresponds to the stored energy function in Valoroso and Champaney [18] if the damage variable D from their formulation is described as

$$D = \frac{y_1}{1 + y_1}. \quad (24)$$

The aberration from the classical damage variable formulation is motivated by the necessity to define the dual dissipation potential $\phi_{\mathcal{S}}^*$ as a function of the thermodynamic driving forces $\dot{z}$ only, as indicated by (11). An expression of t_n in terms of $\dot{z}$ is needed in order to control the dissipative process by the traction. In the present setting, such a relation can be derived from (23), leading to

$$\langle t_n \rangle_+ = \sqrt{2k_n^+ z_1}. \quad (25)$$

This result is exploited in the definition of the overstress function

$$\varphi_n(\dot{z}) = \left\langle \sqrt{2k_n^+ z_1} - \tau_n^c(z_2) \right\rangle_+ \quad \text{with} \quad \tau_n^c(z_2) = \langle -z_2 - \tau_n^s \rangle_+, \quad (26)$$

where τ_n^c represents the critical traction. Here, z_2 is controlled by the softening potential via

$$z_2 = -\frac{\partial \psi_{\mathcal{S}}^s}{\partial y_2} \leq 0, \quad (27)$$

and $\tau_n^s \geq 0$ is introduced in order to attain a stop in the evolution of y_2 at some point. Based on the overstress function, the dual dissipation potential is now defined by a viscous regularization with the viscosity exponent $p \geq 1$, the reference rate $\dot{d}_0 \geq 0$ and the reference value $\varphi_0 > 0$ according to

$$\phi_{\mathcal{S}}^*(\dot{z}) = \frac{\dot{d}_0 \varphi_0}{p+1} \left(\frac{\varphi_n(\dot{z})}{\varphi_0} \right)^{p+1}. \quad (28)$$

While this setting clearly satisfies [R1] and [R2], it also ensures that the internal variables evolve if and only if the cohesive force t_n exceeds the limit τ_n^c , as required in [R4]. Note that the viscous regularization is introduced for numerical reasons in view of possible future applications to multi-scale problems but not in order to model rate-dependency. Hence, the regularization parameters are chosen such that the interface behavior is almost rate-independent throughout this work.

Two different softening potentials are investigated in the present study. This is done to illustrate also the possibility to incorporate new softening laws into the presented framework with ease. An overview of all model parameters is given in Table 2.

3.1.1. Softening type A (see Fig. 4)

$$\psi_{\mathcal{S}}^s(y_2) = \tau_0 \int_0^{y_2} (1 + cy)^{-m} dy = \begin{cases} \frac{\tau_0}{c(m-1)} (1 - (1 + cy_2)^{1-m}), & m > 1, \\ \frac{\tau_0}{c} \ln(1 + cy_2), & m = 1. \end{cases} \quad (29)$$

Parameters: $\tau_0 \geq 0, \quad c > 0, \quad m \geq 1.$

3.1.2. Softening type B (see Fig. 5)

$$\psi_{\mathcal{S}}^s(y_2) = \frac{\tau_0 + \tau_1}{c_1} (1 - \exp(-c_1 y_2)) + \frac{\tau_1}{c_2} (\exp(-c_2 y_2) - 1). \quad (30)$$

Parameters⁴: $\tau_0 \geq 0, \quad \tau_1 \in [-\tau_0, +\infty), \quad c_2 > c_1 > 0.$

3.2. Extension to transversely isotropic interfaces

While only mode I behavior was considered in the model presented in the previous section, many applications require a realistic representation of both, mode I and mode II, as well as mixed-mode properties of a cohesive zone. Therefore, the one-dimensional damage SD-CZM is extended towards a description of transversely isotropic interfaces in the following. Transverse isotropy can be observed at cohesive interfaces in many composites, e.g. in fiber or particle reinforced materials with smooth surfaces. For such interfaces, the Helmholtz free energy density depends on both, the normal interface opening δ_n , and the tangential interface opening δ_t , according to

$$\psi_{\mathcal{S}}(\delta, \hat{y}) = \psi_{\mathcal{S}}(\delta_n, \delta_t, \hat{y}). \quad (31)$$

Consequently, the traction vector can be decomposed into a normal and a tangential component via

$$\mathbf{t} = \frac{\partial \psi_{\mathcal{S}}(\delta, \hat{y})}{\partial \delta} = t_n \mathbf{n} + t_t \mathbf{m}, \quad t_n = \frac{\partial \psi_{\mathcal{S}}(\delta, \hat{y})}{\partial \delta_n}, \quad t_t = \frac{\partial \psi_{\mathcal{S}}(\delta, \hat{y})}{\partial \delta_t}. \quad (32)$$

The approach followed to capture transversely isotropic behavior is to introduce a second dissipative mechanism, i.e. a second overstress function φ_t , a second critical stress τ_t^c and a second softening potential $\psi_{\mathcal{S}}^{d,t}$, associated with the tangential behavior of the interface. The key issue is then to find a proper way of describing the interaction between the normal and the tangential behavior. More precisely, in order to account for mixed-mode decohesion, a reasonable coupling of the two mechanisms is needed to account for the following considerations:

- [C1] complete separation, i.e. a degradation of both critical stresses τ_n^c and τ_t^c to zero, can be attained by loading in any direction, i.e. also by either purely normal or purely tangential loading;
- [C2] both the (positive) normal and the tangential interface stiffness can degrade simultaneously for loading in any direction;
- [C3] the total work of separation W_{sep} varies continuously and monotonically with the load angle $\alpha = \arctan(\delta_t/\delta_n)$ for proportional processes.

While the coupling considerations [C1] and [C2] can be easily realized within the SD-CZ framework, [C3] turned out to be more challenging. Still, since the requirements summarized as [C3] are directly motivated by experimental observations (see, e.g., [26]), much attention has been put on this aspect. Finally, a transversely

⁴ For every physically reasonable set of parameters with $c_2 \leq c_1$, an equivalent set with $c_2 > c_1$ defining exactly the same potential can be found. Thus, the requirement $c_2 > c_1 > 0$ imposes no restriction on the parameter range.

Fig. 4. Four examples of softening behavior of type A defined by the softening potential $\psi_{\mathcal{S}}^s$ given in (29). Gradients of the softening potential (a) and resulting traction-separation curves (b). The traction-separation curves have been computed with $\tau_n^s = 0$, which yields $\tau_n^s(z_2) = -z_2$.

Fig. 5. Four examples of softening behavior of type B defined by the softening potential $\psi_{\mathcal{S}}^s$ given in (30) with $c_2 = 2c_1 = 10 \mu m^{-1}$. Gradients of the softening potential (a) and resulting traction-separation curves (b). The traction-separation curves have been computed with $\tau_n^s = 0$, which yields $\tau_n^s(z_2) = -z_2$.

isotropic damage SD-CZM accounting for all coupling considerations has been developed. In this model, the Helmholtz free energy density has the form

$$\begin{aligned} \psi_{\mathcal{S}}(\delta, \mathbf{y}) &= \psi_{\mathcal{S}}^e(\delta_n, \delta_t, y_1, y_3) + \psi_{\mathcal{S}}^s(y_2, y_4) \\ &= \psi_{\mathcal{S}}^{e,n}(\delta_n, y_1) + \psi_{\mathcal{S}}^{e,t}(\delta_t, y_3) + \psi_{\mathcal{S}}^{s,n}(y_2) + \psi_{\mathcal{S}}^{s,t}(y_4), \end{aligned} \quad (33)$$

using four internal state variables in total. A separation of the terms associated with the normal and the tangential direction appears in (33). Hence, the formulation of coupling is left to the definition of the dual dissipation potential. The elastic parts of the Helmholtz free energy density are defined by

$$\begin{aligned} \psi_{\mathcal{S}}^{e,n}(\delta_n, y_1) &= \frac{1}{2} \frac{k_n^+}{1+y_1} \langle \delta_n \rangle_+^2 + \frac{1}{2} k_n^- \langle \delta_n \rangle_-^2, \\ \psi_{\mathcal{S}}^{e,t}(\delta_t, y_3) &= \frac{1}{2} \frac{k_t}{1+y_3} \delta_t^2. \end{aligned} \quad (34)$$

As before, elastic degradation in normal direction is characterized by y_1 and, similarly, y_3 is introduced for the tangential stiffness. Again, Eq. (25) holds, and the relation

$$t_t = \sqrt{2k_t z_3} \quad (35)$$

is derived similarly. This is exploited for the definition of the effective tractions

$$\tau_n^{\text{eff}}(z_1, z_3) = \sqrt{2(k_n^+ z_1 + \lambda_n^2 k_t z_3)} = \sqrt{\langle t_n \rangle_+^2 + \lambda_n^2 t_t^2}, \quad (36)$$

$$\tau_t^{\text{eff}}(z_1, z_3) = \sqrt{2(k_t z_3 + \lambda_t^2 k_n^+ z_1)} = \sqrt{t_t^2 + \lambda_t^2 \langle t_n \rangle_+^2}, \quad (37)$$

where the coupling parameters $\lambda_n > 0$ and $\lambda_t > 0$ link the evolutions of the internal variables y_1 and y_3 to each other and ensure that [C2]

will be satisfied. The effective tractions allow to define two over-stress functions similar to elliptic flow rules in bulk material plasticity (see, e.g., [27]), given by

$$\varphi_n(\dot{z}) = \langle \tau_n^{\text{eff}}(z_1, z_3) - \tau_n^c(z_2, z_4) \rangle_+ \quad \text{with} \quad \tau_n^c(z_2, z_4) = \langle -z_2 - \alpha_n z_4 - \tau_n^s \rangle_+, \quad (38)$$

$$\varphi_t(\dot{z}) = \langle \tau_t^{\text{eff}}(z_1, z_3) - \tau_t^c(z_2, z_4) \rangle_+ \quad \text{with} \quad \tau_t^c(z_2, z_4) = \langle -z_4 - \alpha_t z_2 - \tau_t^s \rangle_+. \quad (39)$$

The parameters $\alpha_n > 0$ and $\alpha_t > 0$ couple the evolutions of the internal variables y_2 and y_4 and are introduced in view of [C1]. Though a total of four model parameters for the definition of the coupling might appear a lot, each one is relevant in order to account for all effects listed as [C1]–[C3]. For any proportional loading, one of the two criteria $\varphi_n(\dot{z}) = 0$ and $\varphi_t(\dot{z}) = 0$ is activated first, depending on the load angle and the choice of the model parameters. The coupling parameters λ_n and λ_t should be chosen such that the dissipative process is dominated by the normal criterion for mode I loading and by the tangential criterion for mode II loading.

Based on the previous equations, the dual dissipation potential $\phi_{\mathcal{S}}^*$ for the transversely isotropic model is finally defined as

$$\phi_{\mathcal{S}}^*(\dot{z}) = \frac{\dot{d}_0 \varphi_0}{p+1} \left(\frac{\varphi_n(\dot{z})}{\varphi_0} \right)^{p+1} + \frac{\dot{d}_0 \varphi_0}{p+1} \left(\frac{\varphi_t(\dot{z})}{\varphi_0} \right)^{p+1}. \quad (40)$$

For convenience, the same viscous regularization parameters are chosen for both over-stress functions.

4. Numerical implementation

The numerical implementation of constitutive models can be a challenging procedure due to the pronounced nonlinearity and

the stiffness of the system of differential equations. For the SD-CZ framework presented in Section 2, a mixed incremental approach is proposed. It leads to a simultaneous iteration of the driving forces $\hat{z}$ and of the increments of the internal variables $\Delta\hat{y} = \hat{y}(t_{n+1}) - \hat{y}(t_n)$ over a discrete time step of length $\Delta t = t_{n+1} - t_n$. Therefore the nonlinear differential algebraic (DAE) system

$$\dot{\hat{y}} - \frac{\partial \phi_{\mathcal{S}}^*(\hat{z})}{\partial \hat{z}} = \hat{0}, \quad \hat{z} + \frac{\partial \psi_{\mathcal{S}}(\delta, \hat{y})}{\partial \hat{y}} = \hat{0} \quad (41)$$

resulting from Eqs. (10) and (11) is considered. Using the Backward Euler time integration procedure and introducing the algorithmic abbreviations

$$\Delta t = t_{n+1} - t_n, \quad \delta_n = \delta(t_n), \quad \delta_{n+1} = \delta(t_{n+1}), \quad (42)$$

$$\hat{y}_n = \hat{y}(t_n), \quad \hat{y}_{n+1} = \hat{y}(t_{n+1}), \quad \Delta\hat{y} = \hat{y}_{n+1} - \hat{y}_n, \quad (43)$$

$$\hat{z}_n = \hat{z}(t_n), \quad \hat{z}_{n+1} = \hat{z}(t_{n+1}), \quad (44)$$

the discrete nonlinear system of equations is then

$$\hat{f}(\hat{y}_{n+1}, \hat{z}_{n+1}) = \begin{bmatrix} \hat{f}_y(\hat{y}_{n+1}, \hat{z}_{n+1}) \\ \hat{f}_z(\hat{y}_{n+1}, \hat{z}_{n+1}) \end{bmatrix} := \begin{bmatrix} \hat{y}_{n+1} - \hat{y}_n - \Delta t \frac{\partial \phi_{\mathcal{S}}^*(\hat{z}_{n+1})}{\partial \hat{z}} \\ \hat{z}_{n+1} + \frac{\partial \psi_{\mathcal{S}}(\delta_{n+1}, \hat{y}_{n+1})}{\partial \hat{y}} \end{bmatrix} = \hat{0}. \quad (44)$$

A Newton scheme can be used to solve the nonlinear problem (44). With the abbreviations

$$\hat{K} = \frac{\partial^2 \psi_{\mathcal{S}}(\delta_{n+1}, \hat{y}_{n+1})}{\partial \hat{y} \partial \hat{y}}, \quad \hat{L} = \Delta t \frac{\partial^2 \phi_{\mathcal{S}}^*(\hat{z}_{n+1})}{\partial \hat{z} \partial \hat{z}}, \quad (45)$$

the Jacobian of the nonlinear root finding problem (44) is

$$\hat{J} = \begin{bmatrix} \hat{I} & -\hat{L} \\ \hat{K} & \hat{I} \end{bmatrix}. \quad (46)$$

Making use of the particular structure of the Jacobian, the following update procedure is attained:

$$\Delta\hat{z} = -(\hat{I} + \hat{K}\hat{L})^{-1}(\hat{K}\hat{f}_y + \hat{f}_z), \quad \hat{z}_{n+1} \rightarrow \hat{z}_{n+1} + \Delta\hat{z}, \\ \hat{y}_{n+1} \rightarrow \hat{y}_{n+1} + \hat{L}\Delta\hat{z} - \hat{f}_y. \quad (47)$$

The potential structure of the SD-CZ framework allows for an alternative, particularly elegant time integration procedure using a mixed incremental variational formulation. The method exploits the same conceptual ideas as the one used by Miehe [7] and others for bulk materials (see [8], for an application to multi-scale methods). Therefore, we consider the rate potential

$$\Pi_{\mathcal{S}}^*(\dot{\delta}, \dot{\hat{y}}, \dot{\hat{z}}) = \dot{\psi}_{\mathcal{S}} + \dot{\hat{y}} \cdot \dot{\hat{z}} - \phi_{\mathcal{S}}^*(\dot{\hat{z}}). \quad (48)$$

Assuming integration over a discrete time interval of length Δt and an implicit Euler time integration procedure for the internal variables and the driving forces, the saddle point defined by

$$(\hat{y}_{n+1}, \hat{z}_{n+1}) = \text{Arg} \inf_{\hat{y}} \sup_{\hat{z}} \{ \Delta\psi_{\mathcal{S}} + (\hat{y} - \hat{y}_n) \cdot \hat{z} - \Delta t \phi_{\mathcal{S}}^*(\hat{z}) \} \quad (49)$$

is a consistent approximation of the time-continuous model in a discrete setting.

Since the cohesive model proposed in Section 3 is intended for use in an implicit finite element code such as Abaqus/Standard or Ansys, an algorithmic linearization of the surface tractions is required. Due to the potential structure, the symmetry of the algorithmic stiffness operator $\mathbf{K}_a$ is *a priori* guaranteed. This is favorable as it does not hinder the global stiffness matrix from being symmetric when using the finite element method. The definition of the traction vector in (10) leads to

$$\mathbf{K}_a = \frac{d\mathbf{t}}{d\delta} = \frac{\partial^2 \psi_{\mathcal{S}}(\delta, \hat{y})}{\partial \delta \partial \delta} + \frac{\partial^2 \psi_{\mathcal{S}}(\delta, \hat{y})}{\partial \delta \partial \hat{y}} \frac{\partial \hat{y}}{\partial \delta}. \quad (50)$$

Here, the unknown partial derivative of the internal variables $\partial_{\delta} \hat{y}$ is obtained from the linearization of the root finding problem $\hat{f}$ with respect to the displacement jump δ according to

$$\hat{J} \begin{bmatrix} \frac{\partial \hat{y}_{n+1}}{\partial \delta} \\ \frac{\partial \hat{z}_{n+1}}{\partial \delta} \end{bmatrix} + \begin{bmatrix} \hat{0} \\ \frac{\partial^2 \psi_{\mathcal{S}}(\delta_{n+1}, \hat{y}_{n+1})}{\partial \hat{y} \partial \delta} \end{bmatrix} = \hat{0}. \quad (51)$$

Due to the Schwarz theorem, the relation $\partial_{\delta}^2 \psi_{\mathcal{S}} = (\partial_{\hat{y}}^2 \psi_{\mathcal{S}})^T$ holds. The algorithmic stiffness operator is then

$$\mathbf{K}_a = \frac{\partial^2 \psi_{\mathcal{S}}(\delta_{n+1}, \hat{y}_{n+1})}{\partial \delta \partial \delta} - \frac{\partial^2 \psi_{\mathcal{S}}(\delta_{n+1}, \hat{y}_{n+1})}{\partial \delta \partial \hat{y}} (\hat{I} + \hat{L}\hat{K})^{-1} \hat{L} \left(\frac{\partial^2 \psi_{\mathcal{S}}(\delta_{n+1}, \hat{y}_{n+1})}{\partial \delta \partial \hat{y}} \right)^T. \quad (52)$$

For completeness, an expansion of the second partial derivative of the free energy $\psi_{\mathcal{S}}$ with respect to the displacement jump for the transversely isotropic case is presented. In this case, the tractions are given by

$$\mathbf{t} = \frac{\partial \psi_{\mathcal{S}}}{\partial \delta} = \frac{\partial \psi_{\mathcal{S}}}{\partial \delta_n} \mathbf{n} + \frac{\partial \psi_{\mathcal{S}}}{\partial \delta_t} \mathbf{m}, \quad \text{with} \quad \mathbf{m} = \frac{1}{\delta_t} (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \delta. \quad (53)$$

Thus, the second partial derivative of the free energy with respect to the displacement jump is

$$\frac{\partial^2 \psi_{\mathcal{S}}}{\partial \delta \partial \delta} = \frac{\partial^2 \psi_{\mathcal{S}}}{\partial \delta_n \partial \delta_n} \mathbf{n} \otimes \mathbf{n} + \frac{\partial^2 \psi_{\mathcal{S}}}{\partial \delta_t \partial \delta_n} (\mathbf{m} \otimes \mathbf{n} + \mathbf{n} \otimes \mathbf{m}) + \frac{\partial^2 \psi_{\mathcal{S}}}{\partial \delta_t \partial \delta_t} \mathbf{m} \otimes \mathbf{m} \\ + \frac{\partial \psi_{\mathcal{S}}}{\partial \delta_t} \frac{1}{\delta_t} (\mathbf{I} - \mathbf{m} \otimes \mathbf{m} - \mathbf{n} \otimes \mathbf{n}). \quad (54)$$

5. Examples

5.1. Composite splitting

Unidirectional fiber-reinforced composites show a large strength in the fiber direction. Hence, damage is usually initiated by loading perpendicular to the fibers. Fiber cross-over bridging, leading to an increase of the fracture toughness, is frequently observed in that case. This phenomenon has been examined experimentally by Sørensen and Jacobsen [28,23] in a *Double Cantilever Beam* (DCB) test, which allows to draw inferences about the normal behavior of an interface. Monotonic loading experiments with a cross-head displacement rate of 2 mm min⁻¹ were realized for a unidirectional carbon fiber/epoxy matrix composite. Data from two of these experiments by Sørensen and Jacobsen [23] are reproduced in Fig. 6.

The one-dimensional model from Section 3.1 has been fitted to these results for both, softening of type A and softening of type B.

Fig. 6. Numerical results of the one-dimensional model fitted to experimental data by Sørensen and Jacobsen [23].

In both cases, the initial (or undamaged) elastic stiffness and the parameters of the dual dissipation potential were chosen equally and such that the interface model is almost rate-independent. While moderate changes in the parameters mentioned above have only small impacts on the shape of the traction-separation curves, a proper determination of the softening law is of prime importance in this respect. From Fig. 6 it can be concluded that both types of softening laws are suitable to define a model for fiber cross-over bridging. However, Sørensen and Jacobsen [23] stated that the fracture resistance reaches a steady-state level at $\delta_n = 4$ mm. This effect is captured better by the exponential softening law type B, which should, thus, be preferred.

The elastic degradation of the proposed model is demonstrated by a virtual experiment involving loading–unloading cycles (see Fig. 7). Elastic unloading is observed and the same elastic range is found during reloading, thus confirming that the proposed model is in accordance with the requirements [R4] and [R5] from Section 3.1. Note that the elastic slope at the very beginning of the traction-separation curves is hard to see due to a very high initial value k_n^+ of the elastic stiffness.

5.2. Comparison to theoretical results

A well-known reversible cohesive zone law defined by a single potential was proposed by Xu and Needleman [17]. It was shown by van den Bosch et al. [24] and others that this model is only realistic if the normal and tangential work of separation are assumed to be equal. Therefore, an improvement of the Xu and Needleman model with respect to mixed-mode decohesion was presented by van den Bosch et al. [24] (which cannot be derived from a potential, unfortunately). This model was reformulated with a minor change by Kolluri et al. [29], leading to a more transparent formulation of the model parameters without any change in the shape of the traction-separation response. The revised formulation of the improved Xu and Needleman CZM according to Kolluri et al. [29] is

$$t_n(\delta_n, \delta_t) = \frac{\phi_n}{l_n} \frac{\delta_n}{l_n} \exp\left(-\frac{\delta_n}{l_n}\right) \exp\left(-\frac{\delta_t^2}{2l_t^2}\right), \quad (55)$$

$$t_t(\delta_n, \delta_t) = \frac{\phi_t}{l_t} \frac{\delta_t}{l_t} \exp\left(-\frac{\delta_n}{l_n}\right) \exp\left(-\frac{\delta_t^2}{2l_t^2}\right) \left(1 + \frac{\delta_n}{l_n}\right). \quad (56)$$

Here, the normal and tangential work of separation are denoted by ϕ_n and ϕ_t . The characteristic lengths l_n and l_t are related to the maximum normal and tangential stresses $t_n^{\max}$ and $t_t^{\max}$ via

$$l_n = \frac{\phi_n}{t_n^{\max} \exp(1)}, \quad l_t = \frac{\phi_t}{t_t^{\max} \exp(\frac{1}{2})}. \quad (57)$$

A set of parameters as used by van den Bosch et al. [24] is given in Table 3. The transversely isotropic SD-CZM has been fitted to this reference model using softening laws of type A with $m_n = m_t = 1$. A juxtaposition of the traction-separation surfaces of both models can be found in Fig. 8. The plots in Fig. 8(b) have been obtained for proportional processes where the orientation of the displacement jump vector, i.e. the load angle α , was kept constant throughout each loading process while its length was increased at a constant rate of 0.2 nm s^{-1} . Obviously, the requirement [C1] from Section 3.2 is satisfied, i.e. complete separation is observed for pure mode I and pure mode II loading as well as for all mixed-mode cases. It shall be stressed that while the response surface of the model of van den Bosch et al. [24] is path-independent (i.e. the tractions depend only on the current displacement jump), our model shows a strong path-dependency through the internal variables approach. More precisely, two different loading paths with the same final displacement jump will usually result in different values of the internal variables and therefore yield different tractions. Thus, the results depicted in Fig. 8(b) must be understood as a selection of possible traction-separation curves.

According to [C3], the work of separation W_{sep} is required to vary continuously and monotonically with the load angle α . As mentioned in Section 3.2, this requirement was the main challenge

Fig. 7. Loading–unloading behavior: loading (top left), elastic degradation (bottom left) and traction-separation curves (right).

Table 3

Parameters for the improved Xu and Needleman law taken from van den Bosch et al. [24].

$\phi_n = 1 \text{ J m}^{-2}$	$\phi_t = 2 \text{ J m}^{-2}$	$t_n^{\max} = 180 \text{ MPa} \Leftrightarrow l_n = 2.04 \text{ nm}$	$t_t^{\max} = 120 \text{ MPa} \Leftrightarrow l_t = 10.11 \text{ nm}$
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Fig. 8. Traction-separation behavior observed for proportional loading processes.

Fig. 9. Mixed-mode behavior for proportional loadings (a), two-step loadings with tangential loading up to $\delta_t^{\max}$ first and subsequent breaking by normal loading (b), two-step loadings with normal loading up to $\delta_n^{\max}$ first and subsequent breaking by tangential loading (c).

in the modeling of mixed-mode behavior. The dependence of W_{sep} on α is now compared between the improved Xu and Needleman model and the damage SD-CZM. In addition to the model specified in Table 3, three other ratios of the maximum tractions

$\gamma = t_t^{\max}/t_n^{\max}$ have been analyzed, while the normal and tangential work of separation were not modified. For each ratio γ , the damage SD-CZM has been fitted to the reference model of van den Bosch et al. [24] such that a good agreement was found in the

$W_{\text{sep}}-\alpha$ -relations. From the results depicted in Fig. 9(a) it can be concluded that the requirement [C3] is met and that the reference curves are replicated with only minor deviations. At the same time, the ratios of the maximum tractions are also reproduced with satisfactory accuracy (see Table 4).

In addition to proportional processes with varying load angles, two-step loadings have been studied, where the cohesive zone was first loaded in tangential direction up to a maximum δ_t^{max} and subsequently subjected to normal loading until complete separation was attained, and vice versa (see Fig. 9(b) and (c)). The moderate discrepancy between the models for these loadings is not surprising, since the damage SD-CZM exhibits a strong path-dependency and has only been fitted to the reference curves obtained by proportional loadings. A good qualitative agreement is found for the two-step loadings nevertheless. It shall be emphasized that the unphysical mechanical behavior of the original model of Xu and Needleman, e.g. non-monotonic relations in plots like Fig. 9(b) and (c), as elucidated in van den Bosch et al. [24], is not observed for the damage SD-CZM.

The interaction of normal and tangential behavior is demonstrated in Fig. 10. Two cases with a constant loading rate of 5 nm s^{-1} have been studied. It is observed that both the normal stiffness and the critical normal stress τ_n^c are degraded by a purely tangential loading, and vice versa (cp. [C2]).

5.3. Miniature mixed-mode bending test

Several approaches for the experimental determination of mixed-mode interface properties are found in the literature

Table 4
Overview of the ratios of maximum tractions studied.

	Improved Xu and Needleman model		Damage SD-CZM	
	t_n^{max} (MPa)	t_t^{max} (MPa)	t_n^{max} (MPa)	t_t^{max} (MPa)
$\gamma = 1/3$	225	75	222	78
$\gamma = 2/3$	180	120	179	123
$\gamma = 1$	150	150	157	144
$\gamma = 3/2$	120	180	120	196

[30–34]. A miniature mixed-mode bending test (MMMB test) specially designed for in-situ delamination testing was proposed by Kolluri et al. [35] and an improved layout was presented in Kolluri et al. [25] (see Fig. 11). By variation of the loading position ζ in the MMMB apparatus, the whole range of load angles from pure mode I to pure mode II can be achieved (see Fig. 13(b)).

With the improved MMMB setup, the mixed-mode delamination properties of industrially relevant interfaces of a copper lead frame (CuLF) combined with molding compound epoxy (MCE) have been measured in Kolluri et al. [25], as reproduced in Fig. 12. Bi-layer specimens with a length of 35 mm and a width of 5 mm have been used, where the thicknesses of the upper (CuLF) layer and the lower (MCE) layer were 0.2 mm and 0.5 mm, respectively. In Kolluri et al. [36] and Samimi et al. [37], the experimental data from Kolluri et al. [25] were compared to numerical results from FE simulations of the MMMB test, where a self-adaptive cohesive zone framework was employed. While a Smith-Ferrante cohesive zone law was used for the FE simulations in Kolluri et al. [36], the improved Xu and Needleman model of van den Bosch et al. [24] was deployed by Samimi et al. [37].

In order to demonstrate the applicability of the transversely isotropic damage SD-CZM to realistic FE simulations, an FE model of the MMMB test has been created using the commercial Abaqus/Standard software. The modeling of the bi-layer sample was done in 2d under the plane strain assumption, using linear CPE4

Fig. 11. Schematic illustration of the miniature mixed-mode bending test according to Kolluri et al. [25].

Fig. 10. Effects of tangential loading on normal interface behavior (blue) and vice versa (red). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Fig. 12. Comparison of experimental and numerical results of the MMB test. The reaction force P_{MMMB} at the loading point is plotted against the displacement u_{MMMB} .

elements. To deal with the highly brittle interface, a fine discretization was applied to the region of the interface where crack propagation was expected. Mesh studies have been performed in order to ensure that the solutions show no noticeable mesh-dependency. The surface interaction between both layers was defined by incorporation of the damage SD-CZM into the FE model via a UINTER user subroutine. A simplified type B softening law with $\tau_1^0 = \tau_1^1 = 0$ was used for the damage SD-CZM. For a specification of the boundary conditions, the reader is referred to Samimi et al. [37].

Several loading-unloading cycles have been carried out for different loading positions ζ in the MMB apparatus, using the same

model parameters for the interface law in all cases. The resulting force-displacement curves are plotted in Fig. 12. In the beginning of every loading-unloading cycle it is observed that the reaction force P_{MMMB} increases almost linearly with the prescribed displacement u_{MMMB} . At this stage, the specimen is deformed elastically while the crack does not propagate. The subsequent onset of crack propagation shows up as a distinct knee in the force-displacement curves. An exception is found in the experimental results of the first pure mode I load period. As elucidated by Kolluri et al. [25], the microscopic crack tip was initially less pronounced in this case, leading to the smoother behavior. This also serves as an explanation

Fig. 13. Work of separation for different loading positions computed by evaluation of the energy dissipated in loading cycles of the MMB test (left); relation of the load angle at the CuLF-MCE interface and the loading position of the MMB setup, reproduced from Kolluri et al. [36] (right).

for the comparatively large deviation of the FE results from the experimental data in the first load period.

Since the curve obtained from the mixed-mode experiment for $\zeta = 0.67$ is rather non-smooth, a precise numerical reproduction is difficult. However, the FE results obtained with the damage SD-CZM are at least as close to the experiments as the numerical results obtained with the improved Xu and Needleman CZM by Samimi et al. [37] (not shown) in this case and both other mixed-mode cases. With regard to the mode I experiment, the damage SD-CZM can provide an even better prediction than the improved Xu and Needleman law. For the two loading positions $\zeta = 0.00$ and $\zeta = 0.40$, also numerical results obtained with a Smith-Ferrante CZM are available from Kolluri et al. [36] (not shown). These are very similar to the outcome from the simulations run with the damage SD-CZM. Overall, it is found that the FE simulations relying on the damage SD-CZM are in good accordance with experimental observations.

As pointed out above, the relation between the work of separation and the load angle is of major interest concerning the mixed-mode behavior of cohesive interfaces. Hence, the work of separation has been computed for various loading positions ζ by analyzing the energy dissipated in loading–unloading cycles (see Fig. 13(a)). Again, the results obtained for the damage SD-CZM are in very good accordance with the numerical outcome from Kolluri et al. [36], and, more importantly, a good agreement with experimental data is found in the whole range of loading positions.

6. Summary and conclusions

In this work, the idea of defining constitutive laws by two potentials is applied to the modeling of cohesive zones. Such a potential-based framework is well-established for bulk materials and it is known as GSM. Surprisingly, this rather successful and accepted concept has merely been considered for the modeling of dissipative effects in cohesive zones in a rigorous way. In analogy to the notion of standard dissipative solids, we call the class of constitutive interface laws defined by two potentials *standard dissipative cohesive zones* (SD-CZ).

The SD-CZ framework brings along some favorable aspects with respect to implementation and numerics. For any interface model of this class, the time integration scheme presented in Section 4 can be deployed. Due to the fact that the constitutive behavior is entirely given by the gradients of the potential functions, only these gradients must be adjusted for changes in the model, which allows for modular programming. Thereby, the numerical implementation needs to be done only once for an entire class of cohesive behaviors. Hence, the effort for implementation and testing can be reduced significantly, thus leaving more time for the actual modeling part. Further, the proposed setting ensures unconditional symmetry of the algorithmic tangent operator.

The SD-CZ ansatz clearly imposes restrictions on the interface modeling. More precisely, the dual dissipation potential must be defined as a function of the thermodynamic driving forces only, making a straight-forward formulation of mixed-mode behavior difficult. In fact, none of the established CZM for mixed-mode decohesion can be equivalently reformulated within the SD-CZ framework, which underlines the novelty of the present contribution.

Despite the restrictions mentioned above, mixed-mode decohesion can be captured within the SD-CZ framework by the transversely isotropic damage model presented in Section 3.2. This model describes a complex interface behavior including path-dependency, normal-tangential coupling and a continuous and monotonic relation between the work of separation and the load angle. Further, elastic unloading is captured, and loading–unloading behavior is already incorporated into the potential formulation

such that no special adjustment of the numerical implementation is needed.

The numerous features of the transversely isotropic damage SD-CZM come at the cost of a considerable number of model parameters, and the identification of these parameters can be a challenging procedure. Especially the choice of the softening laws and the coupling parameters can raise difficulties, because the mixed-mode behavior is rather sensitive to those. A systematic investigation on this issue is subjected to further research. Nevertheless, some appropriate sets of parameters have already been identified for the examples presented in Section 5. These examples do not only demonstrate the qualitative properties of the transversely isotropic damage SD-CZM, but also allow for quantitative comparisons to theoretical and experimental results from the literature. It is found that the mixed-mode behavior of a specific improved Xu and Needleman CZM taken from van den Bosch et al. [24] can be represented rather precisely by the potential-based model. Furthermore, the mixed-mode bending test introduced in Kolluri et al. [25] was simulated with the finite element method using the damage SD-CZM. Here it is observed that the experimental results are reproduced with good accordance with a fixed set of parameters for the whole range of mixed-mode cases. In addition to this, the shape of a CZM for fiber cross-over bridging that has been experimentally determined by Sørensen and Jacobsen [23] could be replicated with good accuracy in the one-dimensional case.

A promising application of SD-CZ is seen in multi-scale modeling. Decohesion or debonding is observed in many composite materials and may have a significant influence on the overall material response (e.g. [38–41]). In order to account for these phenomena, homogenization methods should be able to deal with microstructures that include cohesive interfaces. In future works, the reduced-order homogenization scheme developed by Fritzen and Leuschner [8] could be extended to such microstructures. For that, the interface behavior is required to be expressed as a SD-CZM due to the specific variational approach of this homogenization technique. Here, the fact that the variational structure of a SD-CZM is preserved under a change of scale is exploited.

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