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Thermodynamic-based cohesive zone healing model for self-healing materials

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ABSTRACT

This work presents a thermodynamic-based cohesive zone framework to model healing in materials that tend to self-heal. The nominal, healing and effective configurations of continuum damage-healing mechanics are extended to represent cohesive zone configurations. To incorporate healing in a cohesive zone model, the principle of virtual power is used to derive the local static/dynamic macroforce balance and the boundary traction as well as the damage and healing microforce balances. A thermodynamic framework for constitutive modeling of damage and healing mechanisms of cracks is used to derive the evolution equations for the damage and healing internal state variables. The effects of temperature, resting time, crack closure, history of healing and damage, and level of damage on the healing behavior of the cohesive zone are incorporated. The proposed model promises solid basis for understanding the self-healing phenomena in self-healing materials.

1. Introduction

In the past decades, many strides have been made to understand the self-healing mechanism in engineering materials [see Hager et al. [1] for an extensive review]. Self-healing materials have attracted intensive research interest because of their ability to sense and respond to damage and recover the material properties. The development of such self-healing properties is of great potential for providing safer, cheaper, more sustainable and durable materials.

Crack healing reverses the cracking process and recovers partially or completely the material stiffness. Wu et al. [2] reviewed various healing mechanisms such as welding, patching, molecular interdiffusion, thermoplastic additives, photo induced healing, self-healing by nanoparticles and others. For a crack to propagate, the energy released must be equal to or greater than the energy required to create new surfaces in the material. Therefore, to retard crack propagation, energy should be dissipated in the material without extending the existing crack. Most of the proposed self-healing concepts describe healing in a single step either by in situ curing of a new phase or a permanent resealing of newly exposed surfaces. In contrast to the aforementioned mechanisms, healing in biological systems proceed via a multi-step mechanism. For example, the healing mechanism of a cut in the skin relies on fast forming patches to seal and protect the damaged skin followed by a slow regeneration of the final repair tissue [2]. Therefore, the introduction of multi-step healing mechanisms will enhance the performance of newly developed self-healing materials.

Several studies on self-healing materials have placed a great focus on modeling microencapsulation in the last decade [e.g., Brown et al. [3]; Brown et al. [4]; Maiti and Geubelle [5]; Mergheim and Steinmann [6]]. The microencapsulation approach has achieved a high healing efficiency in thermosetting materials [7]. On the other hand, self-healing through the thermally stimulated molecular interdiffusion method proved to be the most sustainable for self-healing thermoplastic materials [8,9] such that in these materials repeated healing of a crack can be achieved. The focus of this paper is on modeling the second type of healing that is driven by intrinsic self-healing mechanisms. Several attempts have been made to model the intrinsic self-healing phenomenon for different materials. These attempts have mainly focused on extending the continuum damage mechanics framework to a continuum damage-healing mechanics framework. For example, Barbero et al. [10] used continuum damage-healing mechanics to model the healing mechanism for fiber-reinforced polymer composites. Abu Al-Rub et al. [11] have extended the classical continuum damage mechanics framework by introducing the natural healing

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configuration, and proposed a time-dependent micro-damage healing model to improve the fatigue life predictions of asphalt concrete. This approach has been later adapted by Voyiadjis et al. [12], Darabi et al. [13] and Mergheim and Steinman [6] for modeling micro-damage healing. Darabi et al. [13] developed a micro-damage healing framework that captures the stiffness and strength recovery in cyclic loading upon the application of rest periods, the nonlinear stress–strain response during unloading, and the jump in tangent stiffness modulus at the unloading–loading point. In order to account for the lack of physical healing variables, Voyiadjis et al. [12] introduced healing variables based on the elastic modulus changes during the damage and healing processes, which is along the same lines of Wool and O'Connor [9]. The aforementioned studies treat healing as the reduction of the damaged area and damage density regardless of the crack propagation or healing mechanisms.

Cohesive zone models bridge the gap between fracture mechanics and continuum damage mechanics. Therefore, as they can be used for modeling crack initiation and propagation, they can also be used to model crack closure and healing. There are many cohesive zone/surface constitutive models that have been proposed to describe fracture of various types of materials [see Elices et al. [14], Chaboche [15], Hui et al. [16], and Park and Paulino [17] for reviews of the cohesive zone approach]. However, to the authors' best knowledge, there has been no cohesive zone/surface model that has been developed using thermodynamics for modeling crack healing. Schapery [18] used continuum mechanics to describe crack closing and bonding of surfaces of linear viscoelastic materials. However, instantaneous healing is assumed and the model did not account for the effect of temperature and resting time that are essential for healing as proved experimentally (Darabi et al. [13]). Maiti and Geubelle [5] developed a cohesive finite element method to model fatigue crack growth retardation in polymers induced by artificial crack closure due to presence of a wedge behind the crack tip. This model is motivated through healing by microencapsulation. Their study quantified the effects of load levels, wedge distance to the crack tip, and wedge stiffness.

In this paper, the laws of thermodynamics along with the principle of virtual power are used to develop a phenomenological cohesive zone healing model (CZHM) that can be used for simulating crack healing in self-healing materials. In this CZHM, the local static/dynamic macroforce balance, the boundary traction, the damage microforce balance, and the healing microforce balance are derived based on the principle of virtual power to incorporate healing in a cohesive zone model. In addition, the damage and healing thermodynamics forces are decomposed into energetic and dissipative components along the same lines of Abu Al-Rub and Darabi [19]. The Helmholtz free energy is used to derive the energetic components whereas the maximum rate of energy dissipation principle is used to obtain the dissipative counterparts. The cohesive traction–separation constitutive equations and the damage and healing evolution laws have been derived based on assuming analytical expressions for the Helmholtz free energy and the rate of energy dissipation.

Notation: Hereafter, first-order tensors are represented in small bold letters while higher order tensors are denoted by capital bold letters, (.) and (:) indicate tensor contraction (i.e. $\mathbf{a}.\mathbf{b} = a_i b_i$ and $\mathbf{A}:\mathbf{B} = A_{ij}B_{ij}$), and the superimposed dot ($\dot{}$) stands for differentiation with respect to time t.

2. Cohesive damage and healing discrete configurations

The idea of a cohesive crack healing model is based on the assumption that the whole crack region can be divided into two parts; the first part is where the crack surfaces are free of tractions whereas the second part is where a distribution of cohesive tractions exists such that this distribution is a function of the separation that is driven by damage and healing internal state variables. Based on this assumption, the damage and healing configurations of a single crack are illustrated in Fig. 1. This is based on the continuum natural configuration that was introduced in Abu Al-Rub et al. [11] and elaborated on by Darabi et al. [13]. Upon resting and/or heating, healing initiates at the crack tips where the bonding stress σ_b due to the high atomistic potential causes the two crack surfaces to merge within the cohesive zone length λ as argued by Schapery [18].

The apparent healing configuration shown in Fig. 1(b), which is obtained through resting/heating the damaged configuration in Fig. 1(a), involves a cohesive zone where healing occurs, crack surfaces where the bonding stress is zero, and an intact (undamaged) material. As the separations $\boldsymbol{\delta}_{\mathrm{N}}$ and $\boldsymbol{\delta}_{\mathrm{T}}$ decrease toward the crack tips, the conjugate tractions ($\mathbf{t}_{\mathrm{N}}$ and $\mathbf{t}_{\mathrm{T}}$) within the cohesive zone increase due to the gain in bond strength (σ_b) and surface energy by the healing mechanism (Fig. 1(f) and (g)). By removing the unhealed crack surfaces from the apparent healing configuration, a fictitious healed configuration is obtained (Fig. 1(c)). Whereas, by removing the healed zones a fictitious damaged configuration is attained (Fig. 1(d)). Upon excluding both the damaged and healed zones from the healing configuration a fictitious effective configuration (Fig. 1(e)) is reached which only contains the intact material and has an effective area less than Fig. 1(c) or (d). One may consider certain transformation hypotheses (i.e. strain, elastic strain energy, and power equivalence hypotheses) to analytically relate the stresses and stiffness moduli in these configurations as has been done in Darabi et al. [13] in the case of many distributed cracks.

3. Thermodynamic framework for constructing a cohesive healing zone constitutive model

In a cohesive zone model $\boldsymbol{\delta}$ denotes the displacement jump vector across the cohesive zone (i.e. separation) and $\mathbf{t}$ denotes the conjugate traction vector in the apparent configuration (i.e. Fig. 1(b)). One can decompose $\boldsymbol{\delta}$ and $\mathbf{t}$ into normal and tangential components as follows (see Fig. 1(f)):

$$\boldsymbol{\delta} = \boldsymbol{\delta}_{\mathrm{N}} + \boldsymbol{\delta}_{\mathrm{T}}, \quad \boldsymbol{\delta}_{\mathrm{N}} = \boldsymbol{\delta}_{\mathrm{N}}\boldsymbol{n}, \quad \boldsymbol{\delta}_{\mathrm{T}} = \boldsymbol{\delta} - \boldsymbol{\delta}_{\mathrm{N}}\boldsymbol{n} \tag{1}$$

$$\mathbf{t} = \mathbf{t}_{\mathrm{N}} + \mathbf{t}_{\mathrm{T}}, \quad \mathbf{t}_{\mathrm{N}} = \mathbf{t}_{\mathrm{N}}\boldsymbol{n}, \quad \mathbf{t}_{\mathrm{T}} = \mathbf{t} - \mathbf{t}_{\mathrm{N}}\boldsymbol{n} \tag{2}$$

where $\mathbf{n}$ indicates the normal to the surface of the crack, and subscripts "N" and "T" indicate the normal and tangential components, respectively. The apparent traction is expressed in terms of the effective traction $\bar{\bar{\mathbf{t}}}$ (Fig. 1(e)) as follows:

$$\mathbf{t}_{\mathrm{N}} = \beta_{\mathrm{N}}\bar{\bar{\mathbf{t}}}_{\mathrm{N}}, \quad \mathbf{t}_{\mathrm{T}} = \beta_{\mathrm{T}}\bar{\bar{\mathbf{t}}}_{\mathrm{T}} \tag{3}$$

where

$$\beta_{\mathrm{N}} = (1 - \bar{D}_{\mathrm{N}})H(\delta_{\mathrm{N}}) + H(-\delta_{\mathrm{N}});$$

$$\beta_{\mathrm{T}} = 1 - \bar{D}_{\mathrm{T}} \tag{4}$$

where $H(x)$ denotes the Heaviside step function such that $H = 1$ for $x \geq 0$ and $H = 0$ for $x < 0$; $\bar{D}_{\mathrm{N}}$ and $\bar{D}_{\mathrm{T}}$ are the effective damage variables defined as:

$$\bar{D}_{\mathrm{N}} = D_N(1 - h_N); \quad \bar{D}_{\mathrm{T}} = D_{\mathrm{T}}(1 - h_{\mathrm{T}}) \tag{5}$$

The internal state variables D_{N} and D_{T} are degradation variables of the normal and tangential cohesive strengths, respectively. They are non-dimensional damage variables representing the damaged fraction of the cohesive bonds and ranging between 0 and 1, such that $D = 0$ indicates no damage and $D = 1$ represents complete damage of the cohesive bonds, i.e. complete debonding. On the other hand, the internal state variables h_{N} and h_{T} are healing variables of