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Finite element implementation and application of a cohesive zone damage-healing model for self-healing materials

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ABSTRACT

Self-healing polymers have attracted intensive research interests during the last two decades for being high-potential sustainable materials for civil, military and aerospace applications. To better understand the self-healing phenomena, there is a need to model the time-and-temperature-dependent intrinsic self-healing mechanism at the micro scale and demonstrate crack initiation, propagation, closure and healing. This manuscript presents the numerical implementation of a phenomenological cohesive zone damage-healing model (CZDHM) for self-healing polymeric materials. The effects of temperature, pressure, resting time, instantaneous healing, history of healing and damage, and level of damage on the healing behavior of the material are incorporated in the model and investigated through parametric studies and numerical examples. Model predictions for healing experiments on a self-healing polymeric material are provided to show the capability of the CZDHM to capture self-healing. The proposed model promises a good starting basis for understanding the self-healing phenomena in self-healing materials.

1. Introduction

Self-healing materials have attracted intensive research interests during the last decade because of their ability to sense and respond to damage and recover partially or completely the material properties. The development and understanding of such self-healing properties is of great potential for providing safer, cheaper, more sustainable and durable materials which can be utilized in the aerospace, defense and electronic industries.

Crack healing reverses the cracking process and recovers partially or completely the material properties. In order to demonstrate crack healing, Fig. 1 shows the healing process of the thermoplastic polymer DurusWhite RGD430 which is a polypropylene-like material with a glass transition temperature of 35–37 °C. The sample is shown in Fig. 1(a) with a total volume of 2 cm^3. The healing ability of this polymer was witnessed under scanning electron microscope (SEM) by observing the closure of microcracks. The sample polymer was produced using a 3D printer. Cracks were created in the sample using a razor blade as shown in Fig. 1(b). Then the sample was clamped and placed inside an oven to heal at 70 °C for 12 h. The experimental procedure is further explained in the Appendix. Fig. 1(c) and (e) displays pictures of cracks before healing whereas Fig. 1(d) and (f) shows that these cracks are partially healed after resting, heating and applying pressure.

There exists a huge body of literature on self-healing materials. Wu et al. reviewed various self-healing mechanisms such as welding, patching, thermoplastic additives, photo induced healing, microencapsulation, and self-healing by nanoparticles

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Nomenclature

Θ_o	fracture energy
$\mathbf{n}$	normal to the interface
$\boldsymbol{\delta}$, $\boldsymbol{\delta}_N$, $\boldsymbol{\delta}_T$	total, normal, and tangential displacement jumps across the interface
$\mathbf{t}$, $\mathbf{t}_N$, $\mathbf{t}_T$	the total, normal, and tangential conjugate tractions
$t_T = \sqrt{\mathbf{t}_T \cdot \mathbf{t}_T}$	the effective tangential traction
Ψ^B and Ψ^I	the bulk and interfacial free energy densities
Φ	the cohesive free energy per unit surface area of the fault
ϕ, D_N, and D_T	the bulk, tensile, and shear damage densities
$\mathbf{C}^e$ and $\mathbf{E}^e$	the right Cauchy-Green elastic strain tensor and the Lagrange elastic strain tensor
$\mathbf{F}^e$	the elastic part of the deformation gradient
$\mathbf{S}$	the elastic stress tensor
Y, Y_N and Y_T	the bulk, tensile, and shear damage forces
Π	the rate of energy dissipation due to damage growth, decohesion, and friction
Π^B	the rate of energy dissipation due to bulk damage growth
G and κ	the shear and bulk elastic moduli
$K_N > 0$ and $K_T > 0$	the normal and tangential elastic moduli of the interface
δ_N^o and δ_T^o	the normal and tangential separations at which interfacial damage starts
δ_N^f and δ_T^f	the normal and tangential separations at which full decohesion occurs
h	the hardening/softening modulus of the interface

[1]. Yet, self-healing materials with intrinsic self-healing behavior received intensive research interests during the last two decades. One example is self-healing through thermally stimulated molecular interdiffusion which involves heating a thermoplastic polymer to above its glass transition temperature and healing occurs with the aid of applied pressure. Fig. 1 explains healing in a thermoplastic polymer through thermally stimulated molecular interdiffusion. This healing mechanism was first reported by Jud and Kausch [2]. They demonstrated the crack healing behavior of Poly-methyl methacrylate (PMMA) by heating fractured specimens to about 5–15 °C above their glass transition temperature T_g. During molecular interdiffusion, two polymer surfaces experience both wetting and diffusion [3–5]. Wetting is a short term healing step controlled by the surface energy where partial healing occurs because the crack surfaces contact and wet each other. Diffusion is a long term healing step that is a function of time, temperature, chemical structure, size of the molecules, and pressure. The thermal interdiffusion healing method proved to be the most sustainable for thermoplastic materials such that in these materials repeated healing of a crack can be achieved [3]. However, in the prescribed method, only non-covalent interactions can be established and no new covalent bonds are formed [6]. Chen et al. developed a thermally reversible covalent cross-linking self-healing material through the Diels-Alder (DA) reaction [6]. A cycloaddition of a multi-diene (multi-furan, F) and multi-dienophile (multi-maleimide, M) was used to prepare a highly cross-linked polymeric self-healing material. When the fractured sample is heated, thermal reversibility is accomplished through the DA reaction where the furan and maleimide moieties reconnect and the fractures mend [6,7]. Chen at al. reported that the exothermic polymerization-cross-linking process of the DA adduct is much faster at higher temperatures, reaching "completion" (95%) in just 3 h at 75 °C [6]. Various studies were conducted to experimentally validate the self-healing ability of DA-based materials [8–11].

The focus of this manuscript is to model self-healing materials that exhibit self-healing capabilities with a focus on identifying the factors which control and contribute to the self-healing behavior in such materials. So far many strides have been made to model the self-healing mechanism in various engineering materials at the continuum level [e.g., 12,13–19]. See Hager et al. [20] for a comprehensive review. The focus of this manuscript is on modeling intrinsic self-healing mechanisms. Multiple 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 [14–16,19]. Initially, Abu Al-Rub et al. extended the classical continuum damage mechanics framework by introducing the zero stress time-dependent natural healing configuration, and proposed a time-dependent micro-damage healing model to describe self-healing [15]. The aforementioned studies treated healing as the reduction of the damaged area and damage density regardless of the crack propagation or healing mechanisms. In order to better understand the self-healing behavior, there is a need to model the intrinsic self-healing mechanism at micro-scale and demonstrate crack initiation, propagation, and closure upon healing. This should be coupled with all factors that affect the self-healing ability of the material such as temperature, pressure, time, and history of damage and healing in the material. To achieve this, we adopt a cohesive zone healing approach. Recently, a simple phenomenological cohesive zone damage-healing model (CZDHM) for self-healing materials has been developed based on the principle of virtual power and the laws of thermodynamics [21,22]. The model incorporated the influence of the intrinsic material properties as well as the external effects such as loading,