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A continuum thermo-inelastic model for damage and healing in self-healing glass materials

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ABSTRACT

Self-healing glass, a recent advancement in the class of smart sealing materials, has attracted great attention from both research and industrial communities because of its unique capability of repairing itself at elevated temperatures. However, further development and optimization of this material rely on a more fundamental and thorough understanding of its essential thermo-mechanical response characteristics, which is also pivotal in predicting the coupling and interactions between the nonlinear stress and temperature dependent damage and healing behaviors. In the current study, a continuum three-dimensional thermo-inelastic damage–healing constitutive framework has been developed for the compliant self-healing glass material with different damage mechanisms, i.e. micro-cracks and micro-pores, taken into account. The important feature of the present model is that different physically-driven evolution kinetics have been unified to represent the distinct inelastic, damage, and healing behaviors associated with the mechanical degradation processes. Coupled with the micro-crack and micro-void models reported in the literature, a continuum description of the healing behavior has been established based on the lower-length scale kinetic Monte Carlo simulations to characterize the local thermal–diffusional bond re-formation process across the fracture interface. The proposed formulations are implemented into finite element analyses and the effects of various loading conditions and material properties on the material's mechanical resistance are investigated.

1. Introduction

The interest in self-healing glass materials emerges from the development of hermetic sealants in solid oxide fuel cells (SOFCs) as a promising clean and efficient energy conversion system (Govindaraju et al., 2009). As one of the most important engineering components that are crucial to the long-term reliability and durability of the SOFC systems, the hermetic gas sealant is intended for preventing gas leakage, avoiding fuel–oxidant crossover, and providing electrical insulation (Singh, 2007). Previous studies show that high-temperature glass joining, compared to other sealing techniques, provides a low-cost and relatively simple sealing method. However, its further implementation in the SOFC stack has been overshadowed by the intrinsic vulnerability of conventional glass seals to brittle fracture upon thermal cycling during which tensile stresses develop as a result of the mismatch of thermal expansion coefficients of different stack components (Liu et al., 2010). The

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newly invented thermally responsive self-healing glass that automatically restores its mechanical integrity at high temperatures is encouraging to many, however, lack of fundamental understanding and predictive capability over its long term mechanical functionality and stability at the extreme cell operating temperatures still pose tremendous challenges to the wider applications of this straightforward engineering concept (Liu et al., 2011b; Mihans et al., 2011). In particular, a quantitative and mechanism-based description of its essential stress and temperature dependent degradation and recovery kinetics remains to be sought-after.

Recent exploration in advanced nonlinear materials has greatly inspired the modeling community in developing mechanism-based mathematical rationale in coupling the interactions between deformation processes and damage responses (Haddag et al., 2009; Li and Xu, 2011; Voyiadjis and Kattan, 2009; Voyiadjis et al., 2004). A microstructure-based mesoscopic approach was adopted to correlate the evolution of highly-resolved sub-features to the global characteristics (Basirat et al., 2012; Kadkhodapour et al., 2011; Shen et al., 2012; Tashman et al., 2005), and discrete cell methods were carried out to supplement the criterion for the mechanical deterioration (Pardoen and Hutchinson, 2000; Xu and Needleman, 1994). However, due to the extreme computational intensity, their direct applicability to practical structural and engineering analyses remains limited.

In contrast, continuum phenomenological description, as a homogenization of the underlying microscopic aspects, provides a numerically efficient alternative to project the most relevant microstructure morphological features onto the macroscopic field (Krajcinovic, 1996; Lemaitre, 1992; Lemaitre and Chaboche, 1985). Mechanical degradation interpreted as the damage density was measured based on the reduction of elastic modulus (Bonora et al., 2005; Brunig, 2003; Horstemeyer and Bammann, 2010; Sciarra, 2012; Voyiadjis and Kattan, 2009; Voyiadjis et al., 2004), where the postcritical behavior of the materials was characterized by the evolution of internal variables that denote the accumulation of inherent imperfections such as mechanically induced cracks and internal pores (Doquet et al., 2013; Karamanov et al., 2010). Further observations and analyses suggest that the multiple physical kinetics involved in the degradation process seldom coincide (Hammi and Horstemeyer, 2007; Lecarme et al., 2011). It is therefore necessary to have a unified model which can rigorously account for each of the cooperative phenomena.

Although previous studies have been extensively devoted to describing the irreversible fracture mechanisms (Eftis and Nemes, 1991; Keralavarma et al., 2011; Stahle et al., 2007), theoretical studies on the progressive mechanical rehabilitation as a result of chemical, physical, or biological activities only began to surface recently in the field of self-healing material development (Cordier et al., 2008; Ji and Li, 2013; Kessler et al., 2003; Li et al., 2012; Plaisted and Nemat-Nasser, 2007). From a thermodynamics perspective, the autogenous mechanical recovery was treated as a process that is contrary to the dissipative phenomena and generalized into a so-called continuum damage–healing mechanics (CDHM) framework, in which healing was postulated to follow a similar potential but inverse to that of the damage process (Barbero et al., 2005; Darabi et al., 2013; Voyiadjis et al., 2011, 2012a).

Up until now, most of the modeling efforts devoted to the SOFC compliant self-healing glasses have been typically focusing on limited and particular material aspects, such as cracking (Nguyen et al., 2006; Stephens et al., 2009) or healing (Singh, 2014; Xu et al., 2012), but not inclusively combined. Since the mechanical performance of the SOFC seal glass materials is evaluated based on their holistic damage resistance and recovery behaviors during thermal loading operation, it is important to develop a unified damage/healing model that can resolve the concurrent cracking, voiding and healing in one framework. The essential purpose of the present study is then to establish such a unified computational infrastructure to capture the unique rate-dependent thermo-mechanical damage and healing behaviors with one set of constitutive descriptions. In light of the multiple physical mechanisms involved in the mechanical degradation typically influencing the damage propagation and annihilation differently (Hammi and Horstemeyer, 2007; Lecarme et al., 2011), different evolution kinetics have been unified to resolve their distinct deformation and stress dependencies and interactions. Coupled with the previously developed micro-cracking and micro-voiding models, a continuous description of the characteristic healing behavior is also informed from the lower-length scale kinetic Monte Carlo simulations of the thermal–diffusional bond re-formation between the fracture surfaces in contrast to the phenomenological postulation (Al-Rub et al., 2010). As a result, mechanical inhomogeneity can be considered to extend the healing analysis beyond specific loading conditions (Houjou et al., 2004; Jud et al., 1981). The visco-elastic-damage–healing mathematical formulation is then implemented into finite element (FE) simulations to include spatial influence into the mechanical analysis of the self-healing glass when subjected to different thermal loading cycles. Effects of various operating conditions and material properties were also numerically investigated and discussed in the subsequent sections.

2. Thermo-inelastic damage–healing constitutive relations

2.1. Kinematics

The temperature-dependent and rate-sensitive mechanical behavior of the glass originates from its amorphous, liquid-like but rigidly bounded molecular structure. Despite the absence of long-range atomic translational periodicity, a high degree of short-range order with respect to local atomic polyhedral is preserved by virtue of the chemical bonding constraints (Hufnagel, 2004; Salmon, 2002) in this class of materials. Low temperatures immobilize the disordered structure and arrest the cooperative relaxation behavior in the time scales of any experimental observation, while heating frees up