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Modeling of mechanical behavior of amorphous solids undergoing fatigue loadings, with application to polymers

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ABSTRACT

An approach suitable for modeling viscoelastic-viscoplastic response with isothermal fatigue damage in amorphous solids is proposed. The theory explicitly accounts for frame-indifference and dependence of the free energy on both the viscoelastic-viscoplastic deformation and fatigue damage in a thermodynamically consistent manner. The damage evolution per se is formulated by utilizing an endurance surface that shifts in an effective stress space independent on damage. The idea is suitable for solids in which the fatigue behavior is ductile, i.e. localized damage during the creation of micro-cracks governs majority (up to 95%) of the total fatigue life. Based on implicit numerical integration, the solution procedure is presented, and its capability for technologically important polycarbonate (PC) polymer is addressed. To simulate the fatigue in real specimens, the approach is implemented in a finite-element program. A microscopic, rectangular region representing a RVE of a test specimen is investigated. Simulations, in accordance with experimental observations, indicate that damage develops in small zones around involved inhomogeneities while majority of the material remains undamaged for most of the fatigue life. The results also show that fatigue life can be predicted using a single point at which fatigue most intensively initiates.

1. Introduction

Fatigue denotes the cyclic deformation behavior of materials that may significantly reduce the service life of engineering components at stress levels well below the nominal yield strength. Manufacturers are interested in the fatigue resistance, especially when the service life is difficult to inspect or fatigue may cause an accident under service. In fact, for a long time, the service failures of engineering components owing to mechanical fatigue have been estimated to be the most dominant cause of remarkable financial losses, Ritchie [45] and Beesley et al. [9]. Moreover, time-consuming and costly testing of long-term fatigue life exposed to environmental conditions and previous operation histories can capitalize capable models and the high computational power currently procurable.

Examples of materials having an excellent combination of strength and toughness are amorphous polymers and amorphous metals or alloys, termed bulk metallic glasses (BMGs). However, amorphous solids, particularly BMGs, are susceptible to cyclic fatigue damage that emerges as a low endurance limit, e.g. Launeya et al. [32] and Sun and Wang [50]. Despite this feature and the motivation above, fatigue failure of amorphous solids has received little attention so far. Instead, many of the recent, appealing approaches have focused on micromechanically based damage evolution under multiaxial static loadings that may cause large deformations but not fatigue failure, Lugo et al. [38], Wang et al. [51], and Engqvist et al. [20]. Much of recent studies has also been dedicated to the research of crack development under arbitrary fatigue loadings, see Sun and Wang [50], Dündar and Ayhan [19], Kanters et al. [30], Hughes et al. [28], and Ding et al. [16]. However, referred fracture mechanics based approaches are not aimed at the crack initiation phase that can encompass the majority (even 95%) of the entire fatigue life, Bhattacharya and Ellingwood [11], Marissen et al. [39], and Janssen et al. [29]. Furthermore, research including multiaxial fatigue data for amorphous solids is nonexistent in literature.

Fatigue failure of amorphous solids is owing to either thermally or mechanically governed mechanisms, see Janssen et al. [29] and Murakami [42]. This paper is focused on the mechanically dominated fatigue that does not influence a marked temperature rise and comes forth at relatively low stress frequencies. Fatigue development under such conditions can be divided into two phases. During the first, initiation phase, failure is typically attributed to

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impurities or deficiencies producing notable stress concentrations, which may exceed the strength limits of the material, as has been noted for polymers Marissen et al. [39], Kanters et al. [30], and Holopainen et al. [25] and BMGs Launeya et al. [32] and Sun and Wang [50]. During repeated loadings, these deficiencies can nucleate and form wide crazes already before the desired service life at stress levels far below the nominal yield strength. The second phase is featured by rapid damage growth owing to the coalescence of matured micro-cracks to form large cracks that finally cause material's brittle failure, Ritchie [45], Lesser [35], Lemaitre and Desmorat [34], and Lawrimore et al. [33]. However, in many amorphous solids, the timespan of the first phase is invariably orders of magnitude greater than the second phase, Ritchie [45], Janssen et al. [29], and Kanters et al. [30].

When dealing with fatigue from low- to high-cycle regimes, a suitable damage rule, in addition to the plasticity model, constitutes a substantive part of the analysis. A multitude of approaches exist for fatigue analysis and can be divided into three main groups: energy, strain, and stress approaches, cf. Bannantine et al. [8] and Ottosen et al. [43]. The stress approach, which has been broadly designed for mechanically governed high-cycle fatigue (HCF), constitutes a backbone of the proposed approach. Abounding of those approaches rely on the fatigue-limit criteria, wherein the fatigue strengths or limits are determined by exploiting a large set of identical cycles. They are also equipped with cumulative damage theories and cycle-counting technics that define the damage increase per cycle, Fatemi and Yang [21] and Ottosen et al. [43]. However, it may be challenging to determine a standard cycle from a complex load spectrum, which results in the cycle-counting approaches being inadequate for weighty practical applications.

A different approach to formulate the fatigue model is based on a continuum mechanics framework benefiting an incremental formalism without measuring damage growth per loading cycles, Ottosen et al. [43], Ayoub et al. [7], Murakami [42], Kanters et al. [30], and Holopainen et al. [25]. Such an approach applied here is a modification of an appealing model originally introduced in Ottosen et al. [43]. Albeit the Ottosen et al. [43] -model is intended for the high-cycle fatigue of metals, its conception is rather general and is suitable for amorphous solids that macroscopically show many similar mechanical and fatigue characteristics, Chaboche [14], Lesser [35], Anand and Gurtin [5], Lugo et al. [38], and Holopainen et al. [26,25]. Against canonical $[1-D]$ effective stress damage concepts, cf. Lemaitre and Desmorat [34], Murakami [42], Wang et al. [51], and Holopainen et al. [25], deformations and stresses are now considered independent on fatigue damage, and damage evolution is formulated by using an endurance surface that shifts in a stress space independent on damage. Owing to this assumption, complex relationship between the deformations and damage as well as challenges in numerical implementation due to a damage-induced stress reduction are not encountered. However, coupling between the fatigue model and the governing constitutive model exists and is treated by using a backstress type of internal variable that explicitly influences both the damage evolution and the plastic flow. The idea is valid for amorphous solids in which the fatigue behavior is ductile, i.e. fatigue damage represents solely the formation of micro-cracks and initial crazing that typically cover most of (over 90%) the total service life, Bhattacharya and Ellingwood [11], Janssen et al. [29], and Lugo et al. [38]. In this phase, damaged regions in the material are small and localized compared to those observed after the formation of large cracks. Thus, damage fields and mechanisms do not represent the macroscopic stress reduction in such a manner as is assumed in classical effective stress damage concepts, Chaboche [14]. Since the inhomogeneous stress reduction due to damage is not considered, the proposed approach allows for the prediction of fatigue life of an entire structural element by exploiting solely a single location at which the repetitive load spectrum causes the most determinative fatigue damage.

After introducing kinematics, subsequent thermodynamic treatment as well as the specific fatigue model mentioned in Sections 2.1,2.4, the approach is demonstrated by introducing specific constitutive equations for technologically important amorphous solid polymers in Section 2.5. To investigate low cycle fatigue (LCF), the constitutive counterpart of the proposed approach is based on large deformations, i.e. the multiplicative decomposition of the deformation gradient into viscoplastic and elastic parts is applied, cf. Arruda et al. [6], Anand and Gurtin [5], and Holopainen and Wallin [27]. Many amorphous solids also show a notable viscoelastic deformation behavior, Chaboche [14], Lawrimore et al. [33], and Kwang [31]. To improve predictions under cyclic loading processes as well as under long-term creep and recovery, the model is augmented by a viscoelastic element that further splits the elastic part of the deformation gradient into a viscous component and a purely elastic component, Bergström and Boyce [10], Drescher et al. [18], and Holopainen [23]. When neglecting viscoelasticity and fatigue, the proposed model reduces to the celebrated 8-chain model, referred to as the BPA (Boyce-Parks-Argon) model, see Boyce et al. [12]. Therefore, the presented thermodynamic treatment involving frame-indifference, force and moment balances is also valid for the BPA model. By the authors' knowledge, such a treatment in that extent has not previously been presented for the BPA model.

The article continues by introducing a numerical treatment of the approach mentioned in Section 2.6. Capability of the approach under different loadings for technologically important polycarbonate (PC) polymer is addressed. Based on a finite-element implementation, fatigue testing is simulated, and the contribution of an amorphous polymer structure, in view of dispersed inhomogeneities, to the localization of fatigue damage is debated in Section 3. The article closes with concluding remarks and avenues for future research.

2. The approach

2.1. Kinematics: deformation

Many amorphous materials exhibit distinct time-dependent behavior and also display nonlinear response during loading and unloading which both repeatedly occur in cyclic fatigue loadings, Lesser [35], Chaboche [14], Dreistadt et al. [17], and Lawrimore et al. [33]. These viscous effects show up as creep and relaxation and are due to a microstructure that needs a relaxation time to attain its equilibrium state after deformation. Representative materials are many polymers that show both the viscoelastic and viscoplastic behavior, Chaboche [14], Lawrimore et al. [33], and Kwang [31].

Although viscoelastic deformation is considered low in certain amorphous solids including BMGs, Anand and Gurtin [5], their microstructure also indicates both viscoelastic and viscoplastic behavior (decrease in atomic mobility) of which impact inevitably increases under cyclic fatigue processes owing to factors such as ratcheting and temperature rise, Sun and Wang [50]. To ensure the model's ability to follow the viscous deformation behavior under such conditions as well as under creep and recovery, also the elastic deformation is considered viscous, cf. Chaboche [14], Dreistadt et al. [17], and Holopainen [23].

Deformation of a solid body at time $t \in \mathbb{R}^+$ is defined by the mapping $\boldsymbol{y} : \boldsymbol{X} \mapsto \boldsymbol{x}$ where $\boldsymbol{X} \in \mathfrak{B}$ and $\boldsymbol{x} \in \mathfrak{b}$ are arbitrary material points of the bodies $\mathfrak{B}$ and $\mathfrak{b}$ given in the reference and current deformed placement, respectively.

Based on the Kröner-Lee decomposition, the decomposition