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Research Paper

Anisotropic constitutive model incorporating multiple damage mechanisms for multiscale simulation of dental enamel

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ABSTRACT

An anisotropic constitutive model is proposed in the framework of finite deformation to capture several damage mechanisms occurring in the microstructure of dental enamel, a hierarchical bio-composite. It provides the basis for a homogenization approach for an efficient multiscale (in this case: multiple hierarchy levels) investigation of the deformation and damage behavior. The influence of tension–compression asymmetry and fiber–matrix interaction on the nonlinear deformation behavior of dental enamel is studied by 3D micromechanical simulations under different loading conditions and fiber lengths. The complex deformation behavior and the characteristics and interaction of three damage mechanisms in the damage process of enamel are well captured. The proposed constitutive model incorporating anisotropic damage is applied to the first hierarchical level of dental enamel and validated by experimental results. The effect of the fiber orientation on the damage behavior and compressive strength is studied by comparing micro-pillar experiments of dental enamel at the first hierarchical level in multiple directions of fiber orientation. A very good agreement between computational and experimental results is found for the damage evolution process of dental enamel.

1. Introduction

Dental enamel exhibits both high strength and high toughness simultaneously in spite of a high volume fraction of fibrous hydroxyapatite (90%), a mineral with generally brittle fracture behavior (Fratzl and Weinkamer, 2007). Many studies on the structure–property relationship reveal that nano-sized mineral fibers aligned in a staggered manner in the hierarchical microstructure lead to extraordinary mechanical properties (Chen et al., 2012; Bechtle et al., 2012). Recently, many groups mimic the building principle of dental enamel for developing bio-inspired nano-composites for high performance components (Chen and Pugno, 2013; Espinosa et al., 2009; Humburg et al., 2014). For this purpose, micromechanical models have been proposed and developed to

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clarify the relationship between the unique microstructure and the high damage resistance of enamel (An et al., 2015; Scheider et al., 2015).

Due to the anisotropy of the microstructure and complex damage mechanisms, the deformation and damage modeling of dental enamel are still challenging tasks. Most research efforts focus on modeling the deformation and damage behavior under uniaxial tensile loading perpendicular to the fiber direction (Jäger and Fratzl, 2000; Gao et al., 2003; Bar-On and Wagner, 2011). However, enamel is mainly loaded by compressive and shear forces during mastication and chewing cycles (Yilmaz et al., 2015). Furthermore, the orientation of mineral fibers strongly depends on the location in the enamel and the hierarchical level. Therefore, the investigation of the deformation and damage behavior under compressive loading in fiber direction and inclined to the fiber is crucial for understanding the structure–property relationship of enamel. In addition, linking microstructural characteristics to the macroscopic behavior is necessary for simulating the (homogenized) mechanical response of enamel at higher hierarchical levels and estimating the critical loading of components made by bio-inspired nano-composites. To this end, in the present work, an anisotropic damage model is developed in the framework of continuum damage mechanics and validated by a 3D micro-mechanical model under different tensile, compressive loadings.

In recent years, extensive experimental and computational studies at different length-scales contributed to describe the correlation between high damage tolerance and micro-structural features of enamel, e.g., the aspect ratio of mineral fiber, the fraction of protein, the arrangement of the mineral fiber, as well as the hierarchical structure (Bargmann et al., 2013; An et al., 2012; Bechtle et al., 2010). Barthelat (2014) elaborated a step-by-step approach to design and optimize staggered composites by employing a periodic micro-mechanical model including a failure criterion for the mineral fiber based on fracture mechanics. Lu et al. (2012) introduced a monoclinic anisotropic model based on a 3D micromechanical analysis, which takes into account the orientation changes of the hydroxyapatite crystals and their spatial elastic property variations. An et al. (2012) performed multiscale numerical simulations and found that the non-uniform arrangement of mineral crystallites in prisms enhances the energy dissipation and retains sufficient stiffness for the outer enamel. The majority of these models focused on modeling tensile behavior of enamel based on the small deformation theory. Very limited effort was dedicated to investigate the influence of the mineral fiber orientation on the damage behavior and strength of enamel in the framework of finite deformation. However, this is important for developing a general 3D constitutive model of enamel and must be taken into account to accurately predict the damage accumulation process at different hierarchical levels.

Since dental enamel can be regarded as a fiber reinforced bio-composite with a hierarchical structure, constitutive models for nonlinear anisotropic deformation behavior of fiber reinforced materials in the finite deformation regime can be applied. In the past decades, a large number of phenomenological hyperelastic models have been proposed (Ogden, 1972; Yeoh, 1993; Ehret and Itskov, 2009) for modeling the deformation and damage behavior of bio-composites. deBotton et al. (2006) proposed a transversely isotropic hyperelastic model accounting for material response under out-of-plane and in-plane shear loading modes. Peng et al. (2006) introduced a new term accounting for the fiber–matrix interaction into the strain energy density function. Gasser et al. (2006) developed a hyperelastic potential depending on direction dependent invariants for transversely isotropic material, in particular soft biological tissues. Guo et al. (2014) demonstrated a numerical homogenization approach for predicting the overall mechanical response of the composite under different loading conditions.

In order to simulate the damage behavior of fiber-reinforced composites, continuum damage mechanics has widely been applied to describe the damage accumulation process in different damage modes (Chaboche et al., 1995; Lapczyk and Hurtado, 2007; Maimí et al., 2007; Peña, 2011; Mengoni and Ponthot, 2015; Vasiukov et al., 2015). However, there exists no model capturing the features of matrix damage, fiber damage and interface debonding simultaneously and their interactions with sufficient accuracy. In the present work, an anisotropic damage model is proposed in the framework of finite deformation mapping (i) debonding of interface between mineral fiber and protein, (ii) damage of matrix and (iii) breaking of mineral fibers. A hyperelastic model that describes the nonlinear deformation behavior under various loading condition builds the basis for a proper damage model. Particularly, the influence of tension–compression asymmetry and fiber–matrix interaction on the deformation behavior of dental enamel is studied in 3D micromechanical simulations.

The damage process incorporating different damage mechanisms is studied numerically for dental enamel as a role nano-composite with high and low fiber aspect ratios, which involve two typical failure mechanisms, i.e., the breaking of the fiber (for high aspect ratio) and degradation of interface and matrix (for low aspect ratio). The present model is applied to the first hierarchy level for investigating its predictive capability. Further, the simulation results are compared to experimental results from micro-cantilever beam and micro-pillar experiments. Finally, the effect of the fiber orientation on the damage behavior and compressive strength is investigated.

The novel homogenized damage model, which is developed based on RVE simulations, is able to predict the averaged behavior of the microstructure and take into account the different failure mechanisms by means of distinct damage variables as internal variables. The numerical homogenized approach presented in this work can be applied to higher hierarchical levels for efficiently studying structure–property relationship at higher hierarchical levels and the role of the hierarchical level on the damage-tolerance behavior, since dental enamel can be regarded as a bio-composite with a self-similar structure at each hierarchical level.