Computational Materials Science 79 (2013) 390–401

Contents lists available at SciVerse ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Towards bio-inspired engineering materials: Modeling and simulation of the mechanical behavior of hierarchical bovine dental structure

Swantje Bargmann [a,b,*], Ingo Scheider [a], Tao Xiao [a], Ezgi Yilmaz [c], Gerold A. Schneider [c], Norbert Huber [a]

[a] Helmholtz-Zentrum Geesthacht, Institute of Materials Research, Materials Mechanics, Geesthacht, Germany
[b] Institute of Continuum Mechanics and Material Mechanics, Hamburg University of Technology, Germany
[c] Institute of Advanced Ceramics, Hamburg University of Technology, Germany

ARTICLE INFO

Article history:
Received 7 February 2013
Received in revised form 23 May 2013
Accepted 10 June 2013
Available online 19 July 2013

Keywords:
Bovine teeth
Dental enamel
Cohesive zone model
Size effect
Fracture behavior

ABSTRACT

Dental enamel is the outermost layer of a tooth crown consisting of a hierarchical and graded structure. Approx. 85 vol.% of enamel consist of the hydroxyapatite mineral, the rest being protein and water. This contribution is concerned with the modeling and computation of the mechanical behavior, in particular with the failure, of the enamel of a bovine tooth. For the underlying model description, we resort to a non-linear Neo–Hookean model for the mineral and to the Arruda–Boyce model for the protein, in combination with a cohesive zone approach. The model accounts for non-linear, large-deformation kinematics and softening at the first level hierarchy, and it is validated against experimental data. The numerical implementation is carried out with the help of the finite element method. Here, we resort to a three-dimensional cohesive zone model which maps cracking of the mineral fibers as well as debonding between the mineral fiber and the protein. A complex microstructure representing bovine enamel is studied in the numerical examples. The results capture major features of the physical experiments, such as non-linear stress–strain behavior, stiffness and failure strength.

1. Introduction

Motivated by the fascinating mechanical properties of mineralized biological hierarchical materials, such as bone, dentine enamel or wood [1–3], research on the synthesis of biomimetic hierarchical organic/inorganic materials has been going on worldwide since about two decades. Most techniques are based on self-assembly [4–7] and are restricted to only one level of hierarchy. Among the different methods, freeze casting allows producing materials very similar to nacre with distinguished fracture toughness [8,9]. However, for freeze casting the first level of hierarchy is limited in the order of 1–10 μm.

The Collaborative Research Center SFB 986 "Tailor-Made Multi Scale Materials Systems – M^3", which has been established in Hamburg recently, aims at the synthesis of a self-similar hierarchical material with the first level of hierarchy well below 1 μm and a second level of hierarchy in the range of 1–10 μm. First results on the assembly of the first level of hierarchy have been published recently [10]. By adding another level of hierarchy, the question of the optimal design with respect to geometry and mechanical properties arises. The additional degrees of freedom result in a rather low chance of producing a material with improved properties based on an empirical approach alone.

To overcome this problem, it is important to understand and correctly predict the mechanisms of deformation and fracture of a material having more than one level of hierarchy. It is therefore crucial to start identifying the relevant properties and geometrical features of an existing hierarchical material on each level of hierarchy. This approach provides the required insight into the function of soft and hard phases as well as the interfaces in between and, furthermore, delivers a validated modeling approach. In the following, dental enamel is used as an optimized hierarchical material. A model is built for the first level of hierarchy based on the behavior of the real material, representing the fundamental building block for the next level.

Dental enamel is a load-bearing natural biocomposite, which has evolved to resist fracture and wear. The most striking behavior of enamel from the material scientists' point of view is its longevity in the existence of cracks (under mastication stresses up to 2.5 GPa) in spite of its high mineral volume content. The mechanisms hindering the brittleness of this highly mineralized tissue have been mostly attributed to its hierarchical structuring and also its nanocomposite nature consisting of soft organic matter. For instance, the investigations on the structure–mechanical property relation of enamel could aid to develop human body armor [11], or aid for a better selection of dental restoratives [12].

* Corresponding author at: Helmholtz-Zentrum Geesthacht, Institute of Materials Research, Materials Mechanics, Geesthacht, Germany.
E-mail address: swantje.bargmann@tu-harburg.de (S. Bargmann).

0927-0256/$ - see front matter © 2013 Published by Elsevier B.V.
http://dx.doi.org/10.1016/j.commatsci.2013.06.028

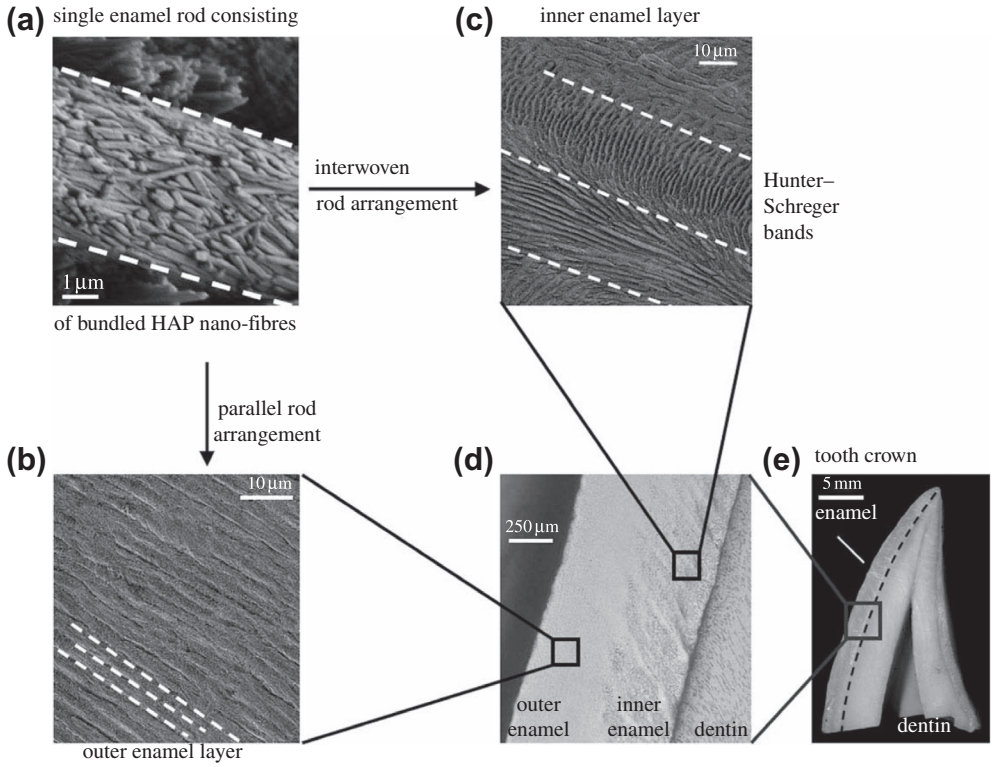

Fig. 1. Hierarchical structure of bovine enamel. Picture taken from Bechtle et al. [23]. (a) Single enamel rod consisting of bundled HAP nano-fibers (level 1: intra-rod). (b) Outer enamel layer with parallel rod arrangement (level 2: multiple rods). (c) Inner enamel layer with interwoven rod arrangement (level 3: Hunter–Schreger bands). (d) Enlarged figure of the outer and inner enamel layer. (e) Bovine teeth cross-section.

In this work, we formulate a mathematical thermodynamically consistent model for the material behavior of dental enamel of bovine teeth which accounts for: (i) size effects, (ii) non-linear elasticity, (iii) softening and (iv) different fracture mechanisms. In this work, the mechanical behavior of the representative volume element (RVE)[1] is simulated representing the microstructure of the first hierarchy level based on Scheider et al. [15,16].

The three-dimensional cohesive zone approach accounts for two failure modes: breaking of the mineral fiber and debonding of the interface between the mineral and the protein. We validate our model against experimental data. The model correctly predicts a size-dependent stress–strain response and different failure modes.

2. Dental enamel of bovine teeth

Dental enamel, the hard protective layer of the tooth crown, is a naturally occurring but a non-vital biological tissue. It has to survive millions of chewing cycles under complex stress state conditions in the oral environment of the host even in the existence of severe internal cracks and flaws [17,18]. In order to meet this functional requirement enamel should possess damage tolerance capability as evidenced in recent studies [19–24], which has been mainly attributed to the complex hierarchical and graded arrangement of its fiber-like mineral crystals and organic constituents.

The hierarchical organization of bovine enamel, which is very similar to human enamel, can be characterized in 3 different levels, see Fig. 1. The simplest and smallest structural units are hydroxyapatite (HAP) nano-fibers glued by proteins (level 1). At the next level of hierarchy HAP nano-fibers are grouped together to form micron-scale structures known as "enamel rods" (level 2) with a diameter of about 5 µm. These rods are covered by organic layers [25]. The rods arrange in a straight and parallel fashion in the layer close to the outer surface (outer enamel); however, in the inner layer close to the dentin (inner enamel), groups of rods with same orientation decussate each other periodically forming so-called "Hunter–Schreger bands" (level 3). The width of the bands vary between 20 and 50 µm in bovine enamel. The mechanical properties such as the stress–strain behavior or the elastic modulus (see, e.g., [23]) differ greatly on the different hierarchical levels.

The mechanical functionality of enamel's hierarchical structure is an on-going issue. For example, measurements with Vickers indents (Indentation Crack Lengths Method, [26]) gave a small fracture toughness of the order of 1 MPa $m^{1/2}$ [27–29]. This led to the prevailing opinion that enamel is a brittle material. More recently, R-curve measurements [20,22] revealed that the fracture resistance of enamel rises up to 4 MPa $m^{1/2}$ due to its graded structure and toughening mechanisms operating on all hierarchical levels [19]. This offers an additional explanation for the well-known crack arrest at the dentin enamel junction [30]. In addition to a drop in the stress intensity factor for a crack crossing the dentin enamel junction due to an elastic modulus drop of a factor three, the toughness of long cracks in enamel is equal or may even surpass the toughness in dentin [22]. A quantitative mechanical understanding of these effects is only possible, if the complex hierarchical microstructure of enamel is modeled. First steps in this regard are Gao's self-similar concepts [31]. In this paper, we intend to be closer to the real microstructure of enamel, which necessitates a numerical simulation based on the microstructure.

[1] In general, the existence of an RVE is questionable as soon as localized material degradation and damage occurs, see e.g. [13,14] – if the damage behavior is incorporated into the continuum model. In a cohesive model, damage and deformation are modeled by two different models, a continuum model and a cohesive model. Since the fracture process zone for the cohesive model is reduced to zero, the absolute size of it is incorporated in the model parameters and not in the geometry. The continuum model then only contains deformation. This model has been published in [57,58]