

Role of crystal arrangement on the mechanical performance of enamel

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ABSTRACT

The superior mechanical properties of enamel, such as excellent penetration and crack resistance, are believed to be related to the unique microscopic structure. In this study, the effects of hydroxyapatite (HAP) crystallite orientation on the mechanical behavior of enamel have been investigated through a series of multiscale numerical simulations. A micromechanical model, which considers the HAP crystal arrangement in enamel prisms, the hierarchical structure of HAP crystals and the inelastic mechanical behavior of protein, has been developed. Numerical simulations revealed that, under compressive loading, plastic deformation progression took place in enamel prisms, which is responsible for the experimentally observed post-yield strain hardening. By comparing the mechanical responses for the uniform and non-uniform arrangement of HAP crystals within enamel prisms, it was found that the stiffness for the two cases was identical, while much greater energy dissipation was observed in the enamel with the non-uniform arrangement. Based on these results, we propose an important mechanism whereby the non-uniform arrangement of crystals in enamel rods enhances energy dissipation while maintaining sufficient stiffness to promote fracture toughness, mitigation of fracture and resistance to penetration deformation. Further simulations indicated that the non-uniform arrangement of the HAP crystals is a key factor responsible for the unique mechanical behavior of enamel, while the change in the nanostructure of nanocomposites could dictate the Young's modulus and yield strength of the biocomposite.

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1. Introduction

As the outermost hard tissue of teeth, enamel possesses a complex hierarchical structure [1]. On the micron length scale, enamel is a biocomposite consisting of keyhole-like prisms with a diameter of approximately 5 μm [2,3] and protein-rich prism sheaths which have a thickness of 800–1000 nm [4] and constitute the boundaries of prisms [5]. The individual prisms also exhibit a composite structure composed of hydroxyapatite (HAP) crystallites embedded in a soft protein layer with a thickness of ~ 2 nm [6,7], which forms the nanostructure of enamel. The HAP crystals have a thickness of 20–120 nm [8–10] and exhibit different orientations within enamel prisms. In the prism head, HAP crystals are parallel to the prism axis, while in the tail, an angle of 60° between the crystal *c*-axis and the prism axis is observed [11]. In regions between the prism head and tail, the *c*-axes of crystals gradually incline to the prism axis with an angle up to 60°.

The microstructure and mechanical performance of enamel have been studied through experimental and numerical approaches.

Owing to the small size, fracture of HAP crystallites is governed by the theoretical strength rather than the crack propagation, which implies that the mineral crystallites in nanocomposites are insensitive to flaws [12]. It was found through the indentation technique that, owing to the high percentage (95%) of minerals in enamel [13], the elastic modulus of enamel was 70–120 GPa [14–16], which is much greater than that for other hard tissues (bone and dentin). While the content of protein is low compared with minerals, it has a significant influence on the mechanical behavior of enamel. He and Swain [17,18] reported that, when enamel was subjected to contact loading, the protein underwent large shear deformation, and the inelastic deformation behavior of the protein resulted in the nonlinear stress–strain response for enamel. Studies by Xie et al. [19,20] revealed that, when the protein became thicker, which was typical in hypomineralized enamel, the ability of enamel to resist inelastic deformation was reduced, providing an explanation for the degraded mechanical properties of hypomineralized enamel [21,22]. Due to the existence of sacrificial bonds, which may rupture when protein experiences large deformation, protein can also lead to the irreversible deformation behavior of enamel [23,24]. He and Swain [10] reported that the indentation stress–strain curve for enamel was similar to that for metals, rather than its major constituents (HAP crystals). The plastic deformation, which was demonstrated

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by the residual impression after unloading, was further revealed. More recently, Ang et al. [25] utilized spherical indenters with different radii to evaluate the indentation stress–strain response for enamel at multiple length scales, and found that the constitutive relationship of enamel was dependent on the length scales. The plasticity and damage caused by microcracking were the primary mechanisms responsible for the inelastic deformation behavior of enamel. Protein also plays an important role in the fracture properties of biocomposites. Thick protein layers could reduce stress concentration at the crack tip, thereby enhancing the fracture toughness of biocomposites [26].

Besides the constituents of enamel, the mechanical performance of enamel is also dependent on the organization of these constituents. Ji and Gao [27] declared that the Young's moduli and shear modulus of biocomposites are highly anisotropic. The staggered arrangement of mineral crystals adopted by natural biological materials leads to high stiffness and strength, and good energy storage abilities [28]. Liu et al. [29] derived analytical solutions of stress and strain distribution for further studying the complex mechanical properties of biological materials. Based on the fact that many biological materials possess hierarchical structures [30–32], Gao [33] and Yao and Gao [34] developed a self-similar hierarchical model to study the mechanical properties of hierarchical biological materials. Based on the theory for hierarchical materials, Bechtle et al. [1] analyzed the experimental data for enamel and concluded that the stiffness, strength and toughness of enamel were functions of levels of hierarchy. An et al. [35] studied the plastic deformation and gradient properties of enamel using nanoindentation and numerical simulation.

As the foundation for enamel, dentin also plays an important role in tooth function. The low modulus and hardness of dentin can reduce stress in teeth [16]. Imbeni et al. [36] conducted indentation experiments on teeth, and found that cracks initiated in enamel propagated through the dentin–enamel junction and stopped in dentin, implying that dentin exhibited strong resistance to crack growth and thereby promoted damage tolerance of teeth. The study by Brauer et al. [37] indicated that it was the asymmetries of stiffness and hardness of dentin that enabled the tooth to resist impact loading effectively.

Previous studies have identified the hierarchical microstructure of enamel and mechanical behaviors of enamel. However, the relationship between the mechanical properties and the HAP crystallite arrangement is still under investigation. For instance, as the high percentage of mineral may lead to brittleness in enamel [38], how does enamel achieve damage tolerance during mastication to retain structural integrity? Why is it the non-uniform arrangement, rather than the uniform arrangement, of HAP crystallites in prisms that is present by enamel? These questions call for a better understanding of the relationship between the structure, mechanical properties and functions of enamel. The primary goal of this investigation is to explore the mechanical advantages of the non-uniform distribution of HAP crystallites, as well as to identify the mechanical design principles of enamel. A series of hierarchical numerical modeling which considered the HAP structure and its orientation at different regions in enamel rods were conducted. The influences of HAP crystal arrangement on the stiffness, energy dissipation and mitigation of fracture are elucidated. The underlying deformation mechanism of enamel under compressive loading is discovered.

2. Methods

Since enamel possesses a hierarchical microstructure, multiscale numerical simulations, i.e. at the nano- and microscales, were conducted.

2.1. Nanocomposite modeling

Enamel is a nanocomposite consisting of hexagonal HAP crystallites and protein, tightly packed and oriented at different angles from the prism head to the tail. The mechanical properties of the nanocomposite can be evaluated by constructing a representative volume element (RVE) and exploring the mechanical behavior of the RVE. In this study three RVEs were considered.

RVE(A) takes into account the imperfection of HAP crystallites, such as the curvature and branch [39]. Wang et al. [40] and Han et al. [41] created an RVE for the nanocomposite ganoine scales of *Polypterus senegalus*, in which the transverse mineral element was introduced to capture the effects of discontinuity of the protein and the irregular arrangement of mineral crystallites. Considering that at the nanoscale enamel and ganoine have identical building blocks, i.e. HAP crystallites and protein, and that the crystallites possess the same volume fraction and geometry in both those biological materials [40], in this study the RVE for ganoine was adopted and referred to as RVE(A) (Fig. 1a).

RVE(B) was accordingly introduced based on the assumption of the regular alignment of HAP crystallites without considering the imperfection of the nanocomposite. This RVE is used to investigate the influence of crystal imperfection on the mechanical properties of enamel.

It is reported that the thickness of crystallites in enamel is 40–50 nm [19,42]. Here, in order to investigate the influence of crystallite thickness (or influence of the volume fraction of minerals) on the mechanical response of enamel, RVE(C), which is also based on the assumption of the regular alignment of HAP crystallites, was developed.

RVE(B) has the same morphology as RVE(C), while the thicknesses of mineral crystallites in RVE(B) and RVE(C) are distinct. As shown in Fig. 1, the protein sheets in RVE(A) become discontinuous due to the introduction of transverse mineral elements, whereas the protein layers in RVE(B) and RVE(C) are continuous. Note that the length for the three RVEs is taken to be 220 nm, which is consistent with the observed value, 100 nm–100 μ m [9,39,43], and the RVEs are also suitable for the case where the HAP crystallite length reaches up to 100 μ m, where the nanocomposite can be considered as a long-fiber-reinforced composite. The thickness for protein in the three RVEs was assigned to be 2 nm, and the HAP crystallite thickness in RVE(A) was taken as 40 nm, while those for RVE(B) and RVE(C) were 50 and 40 nm, respectively [19,42].

2.2. Microscopic modeling

The mechanical properties of enamel can be determined by investigating the mechanical performance of a biocomposite

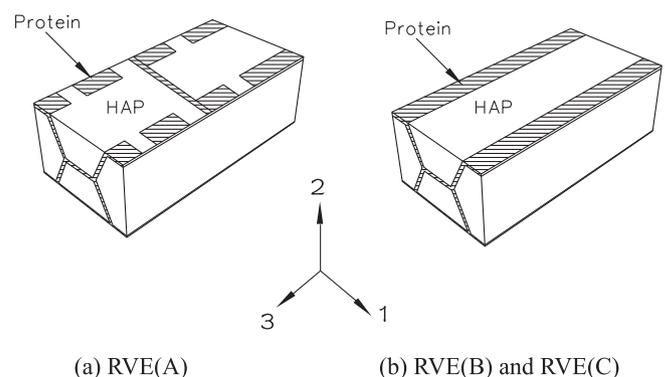


Fig. 1. RVEs for nanocomposites consisting of hexagonal HAP crystallites and protein.

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