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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.

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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