

Fiber Bundle Modeling for Nacre Fracture Simulation

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Abstract

Nacre exhibits phenomenal fracture strength and toughness properties despite its relatively weak material properties. Its work of fracture is about 3000 times greater than that of a single crystal of its constituent mineral. This is surprising because it is a ceramic composite made up of 95% brittle calcium carbonate (CaCO₃) and 5% of a biopolymer material (organic glue). Today, synthetic polymer-matrix composites with such high levels of ceramic fillers do not possess these exceptional combinations of stiffness, fracture strength and toughness. Understanding the mechanisms of such high damage tolerance of nacre will enhance our ability to design novel materials for innovative practical applications. Research on synthesizing such tough materials is currently under intense development at Oak Ridge National Laboratory and elsewhere, since these materials can be used as light-weight body armor and in various defense related applications. This study investigates the fracture properties of nacre using statistical physics based continuous damage Worm-Like Chain (WLC) model. The WLC model represents a realistic force-extension curve of protein molecules. The constitutive law of the organic interface is derived using a fiber bundle model, wherein the force-extension behavior of each of the fibers is described by a WLC of entropic elasticity. Both local and global load sharing fiber bundle models are used to understand the fracture properties of nacre.

Introduction

Nacre composite resembles “brick and mortar” microarchitecture with interlaced ceramic platelets (bricks) separated by soft biopolymer (mortar). To determine what makes nacre so strong, the structure is examined on a nanometer scale. The secret to its phenomenal strength lies within the biopolymer itself. The microstructure consists of millions of organic fibers. Each fiber consists of nano-size modules (bumps). As tension is applied to the platelets, the modules unwind prior to fiber fracture, as shown in Fig. 1. This poster presents a fiber bundle model with Worm-Like Chains (WLC) to represent the biopolymer force-displacement response of nacre.

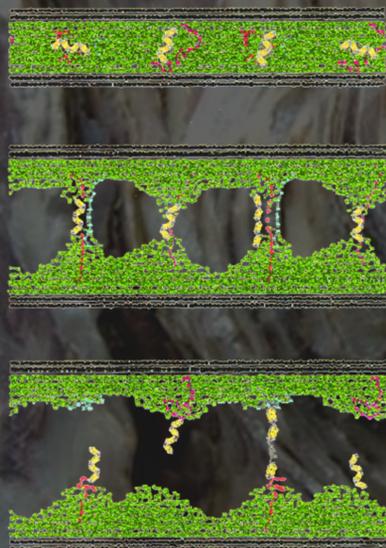


Fig. 1. Schematic example of an organic polymer with modules unwinding before fracture.

Experimental Response of Nacre's Biopolymer

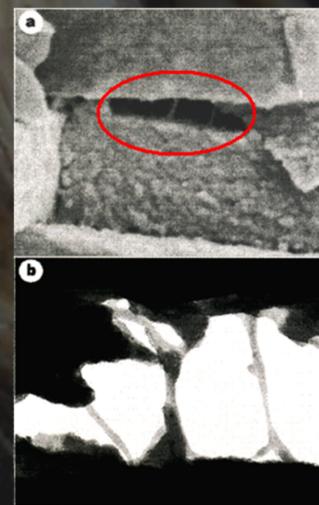


Fig. 2. Abalone nacre platelets and protein fibers under mechanical stress.

Protein fibers between two abalone nacre platelets under mechanical stress obtained from scanning and transmission electron micrographs are presented in Fig. 2. The corresponding mechanical response of the organic interface is presented in Fig. 3. The unfolding events (sawtooth pattern) of the modules of the protein fibers are clearly visible in Fig. 3.

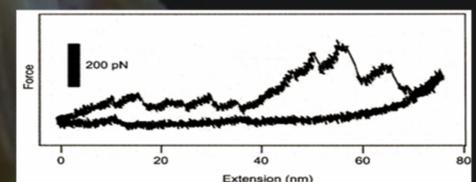


Fig. 3. Force-extension response of organic interface obtained using an atomic force microscope.

Summary of Results

Mechanical response of a single biopolymer fiber response is obtained using an atomic force microscopy (AFM), as shown in Fig. 4. Figure 5 presents the corresponding experimental response of a single protein fiber including the unfolding of the modules (sawtooth pattern). The response of a WLC model is also shown in Fig. 5 and is in excellent agreement with the experimental response.

WLC Model

Mechanical response of a single biopolymer fiber response is obtained using an atomic force microscopy (AFM), as shown in Fig. 4. Figure 5 presents the corresponding experimental response of a single protein fiber including the unfolding of the modules (sawtooth pattern). The response of a WLC model is also shown in Fig. 5 and is in excellent agreement with the experimental response.

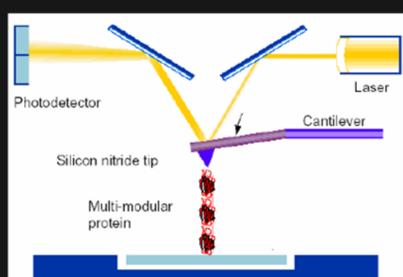


Fig. 4. Atomic force microscopy (AFM) is used to induce unfolding of a single protein fiber.

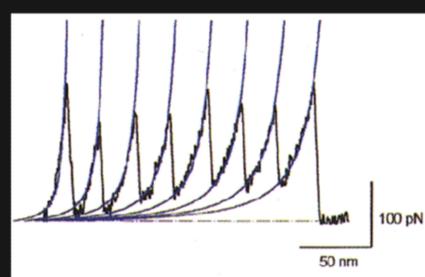


Fig. 5. WLC model used to describe unwinding of a single protein fiber.

➤ Equation used to describe WLC model for a single protein fiber

$$f = \left(\frac{k_B T}{A} \right) \left[\frac{1}{4(1-z/L)^2} - \frac{1}{4} + \frac{z}{L} \right]$$

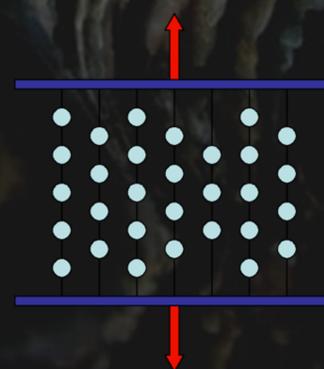


Fig. 6. Schematic of a fiber bundle model with WLC fibers and unfolding modules.

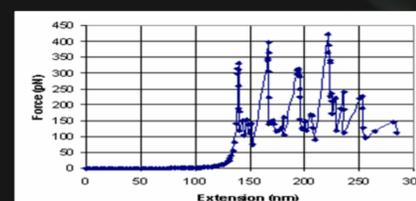


Fig. 7. WLC fiber bundle model simulation of an organic interface.

Figure 6 is a schematic fiber bundle model of an abalone nacre interface shown in Fig. 2. Each of the fibers in Fig. 6 is modeled using a WLC model (Eq. 1). Each fiber has a random number of modules, which unfold at random thresholds. Whenever a module unfolds, the persistence length of the fiber changes thereby changing its WLC response. The numerical response of the fiber bundle model with WLC fibers is shown in Fig. 7, which is in excellent agreement with the experimental response shown in Fig. 3. Figure 8 presents the effect of number of unwinding modules per fiber on the mechanical response of nacre's interface.

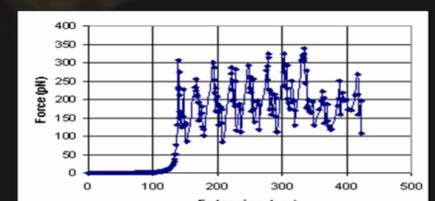


Fig. 8. Effect of number of unwinding modules per fiber on mechanical response of nacre's interface.