Fiber Bundle Modeling for Nacre Fracture Simulation

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http://www.csm.ornl.gov/Internships/rams_06/abstracts/j_fletcher.pdf

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. We consider both local and global load sharing fiber bundle models 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 find out what makes nacre so strong, the structure is examined on a nanometer scale. The secret to it’s 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 is Fig. 1. This poster presents a fiber bundle model with Worm-Like Chains (WLC) to represent the biopolymer force- displacement response of nacre.

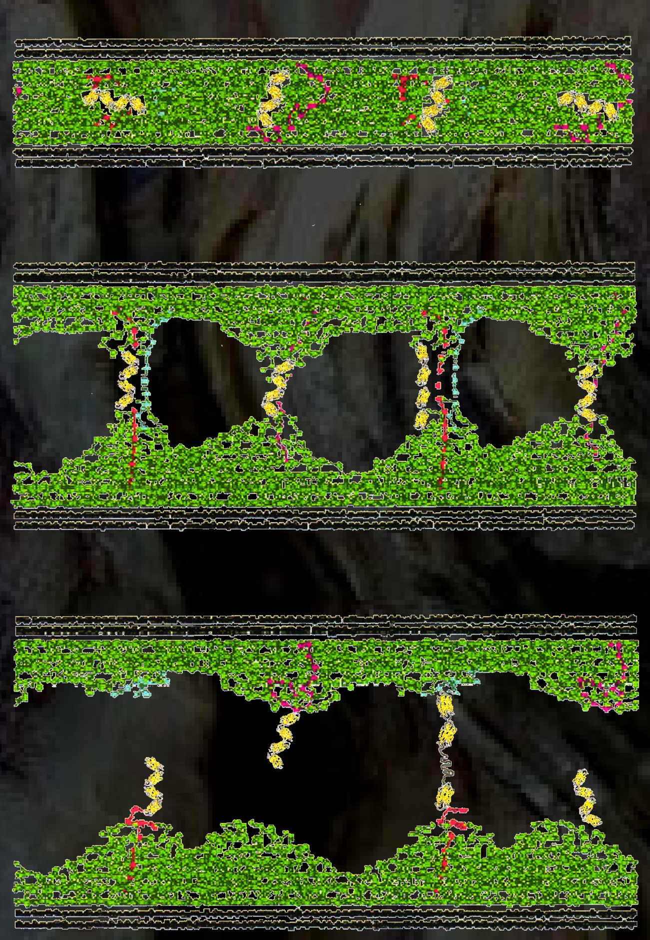

Fig. 1. Schematic example of an organic polymer with modules unwinding before fracture

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.

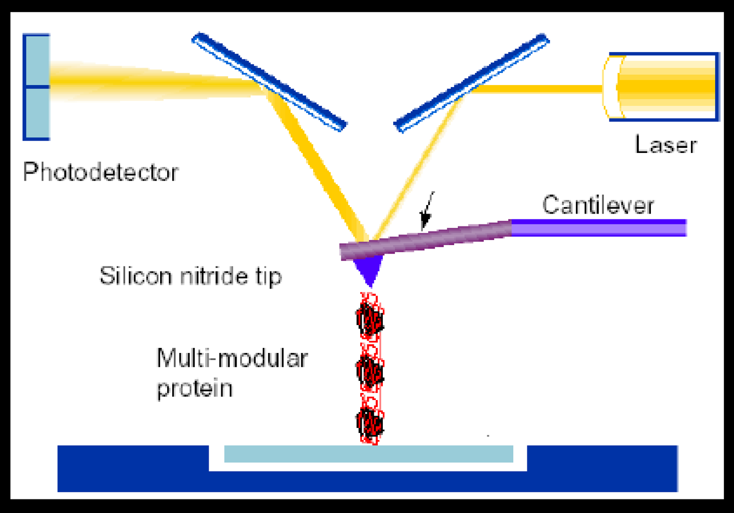

Fig. 4. Atomic force microscopy (AFM) is used to induce unfolding of a single protein fiber

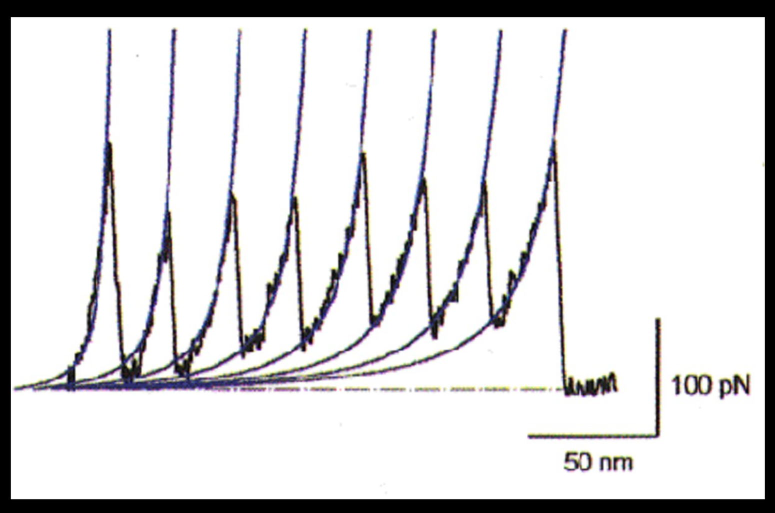

Fig. 5. WLC model used to describe the unwinding of a single protein fiber

- An equation is used to describe WLC model for a single protein fiber

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

Experimental Response of Nacre’s Biopolymer

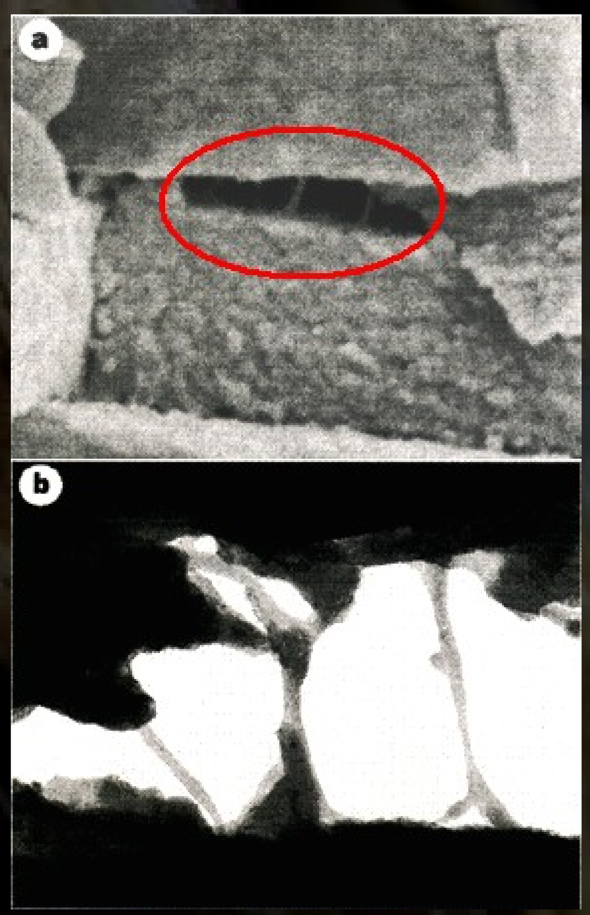

Fig. 2. Abalone nacre platelets and protein fibers under mechanical stress

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.

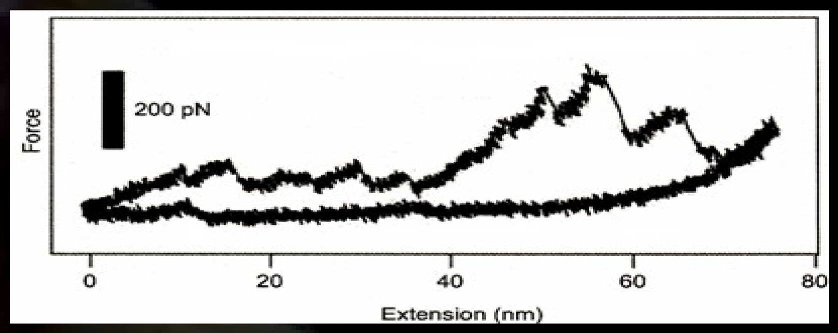

Fig. 3. Force-extension response of organic interface obtained using an atomic force microscope.

Summary of Results

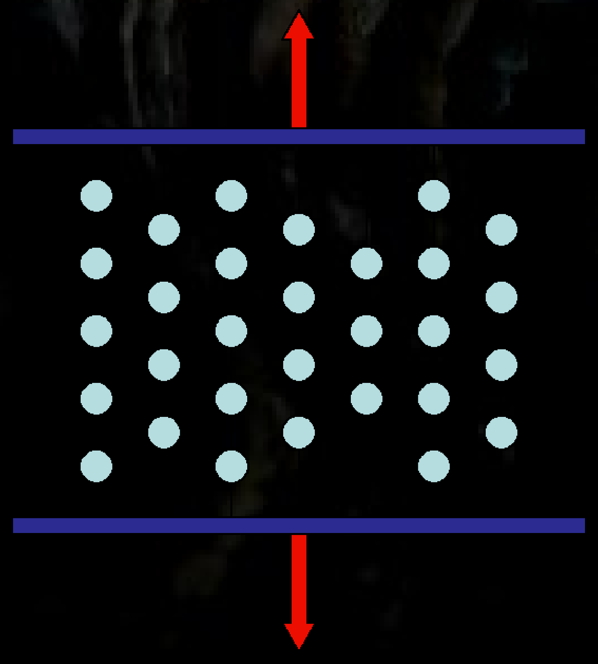

Fig. 6. Schematic of a fiber bundle model with WLC fibers and unfolding modules

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.

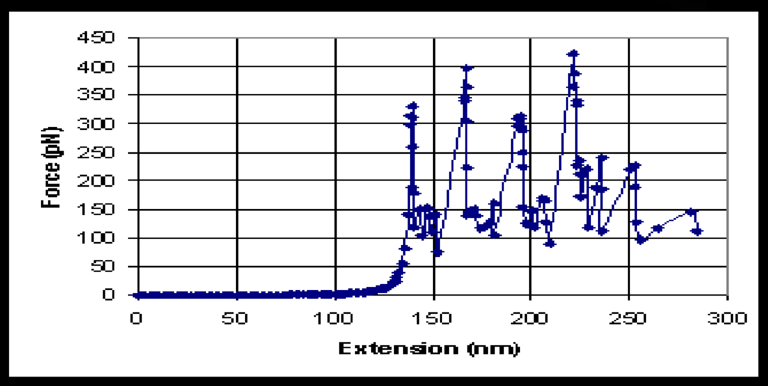

Fig. 7. WLC fiber bundle model simulation of an organic interface

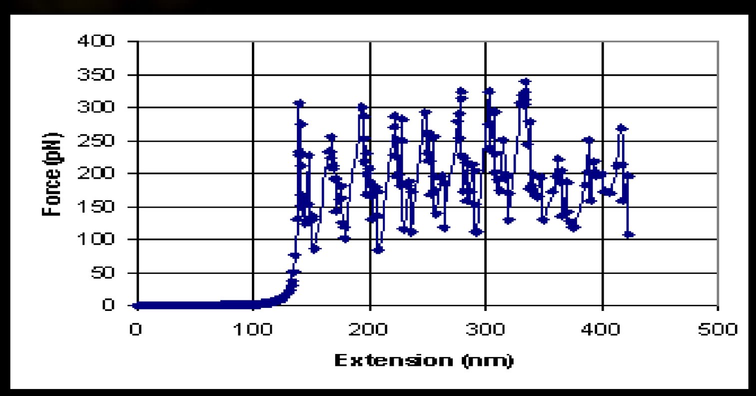

Fig. 8. Effect of number of unwinding modules per fiber on mechanical response of nacre’s interface

The Research Alliance in Math and Science program is sponsored by the Mathematical, Information, and Computational Sciences Division, Office of Advanced Scientific Computing Research, U.S. Department of Energy. The work was performed at the Oak Ridge National Laboratory, which is managed by UT-Battelle, LLC under Contract No. De-AC05-00OR22725. This work has been authored by a contractor of the U.S. Government, accordingly, the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes.

To my mentor, Dr. Nukala, I would like to thank you for use of your research and assisting me in developing my project. I would like to thank my colleague, Ryan Hurd of Hurd Designs© for his assistance on my poster, and special thanks to Debbie McCoy and Dr. Deng for again making this internship possible.

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