UT-BATTELLE

Fiber Bundle Modeling for Nacre Fracture Simulation

Presented to

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Outline

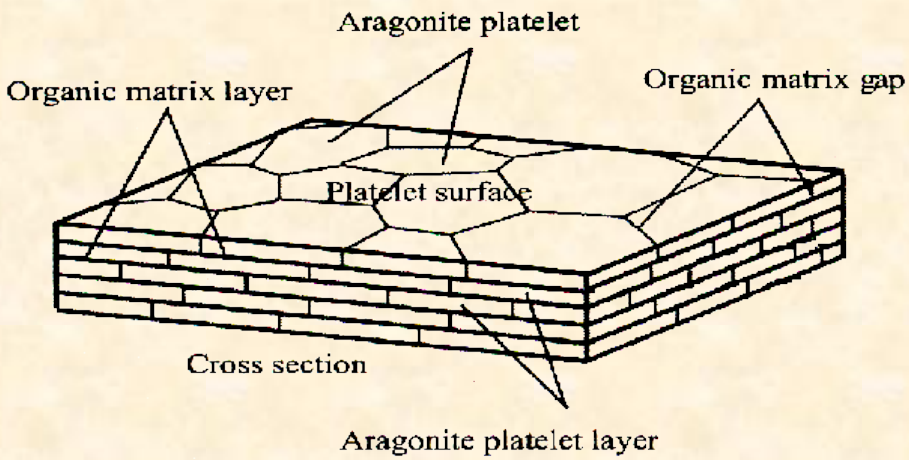
- Background on Nacre
- Motivation for Research
- Scientific Significance
- Experimental Response of Nacre's Biopolymer
- Project Goals
- Worm-like Chain model (WLC)
- Summary of research
- Results

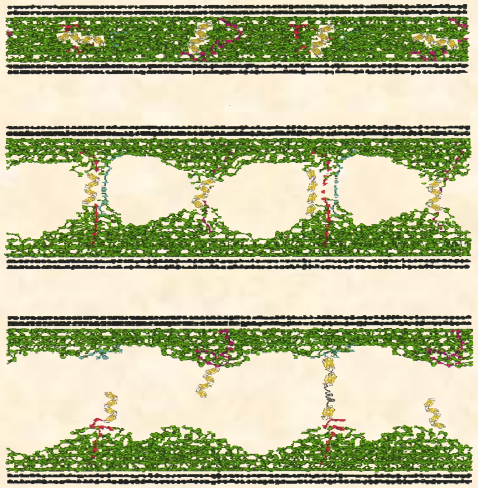
Background on Nacre

- Nacre exhibits phenomenal fracture strength and toughness
- Relative weak material properties
- Ceramic composite made up of 95% brittle calcium carbonate ($CaCO_3$)
- 5% biopolymer material (organic glue)
- Work of fracture is about 3000 times greater than a single crystal of its constituent mineral

Background on Nacre (Continued)

- Resembles "brick and mortar microstructure
- Millions of organic fibers
- Each fiber consists of nano-size modules (bumps)
- Modules unwind prior to fracture





Motivation

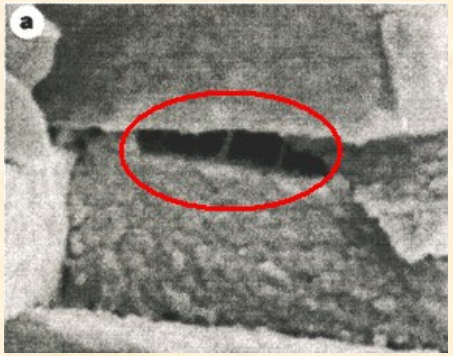
- Synthetic polymer-matrix composites with high levels of ceramic fillers
- Exceptional combinations of stiffness, fracture strength and toughness
- Nanoscopic unwinding of organic fibers

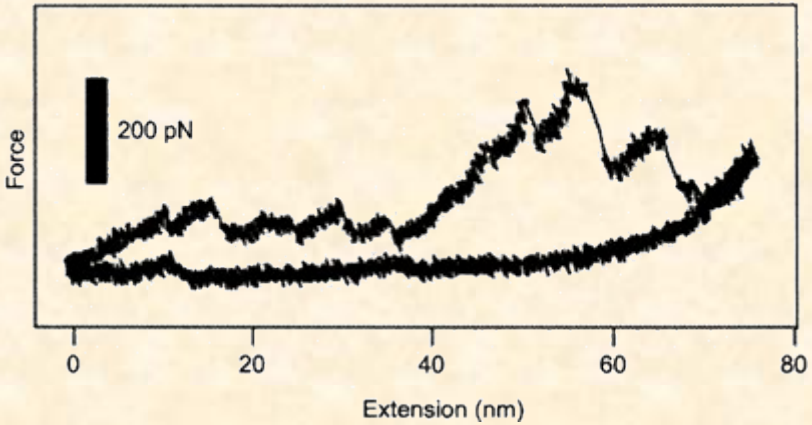
Scientific Significance

- Understand the mechanisms high damage tolerance
- Enhance ability to design novel materials for innovative practical applications
- Materials can be used as light-weight body armor

Experimental Response of Nacre's Biopolymer

- Mechanical stress of protein fibers between two abalone nacre platelets
- Corresponding mechanical response of the organic interface
- Unfolding events (sawtooth pattern) of the modules of the protein fibers



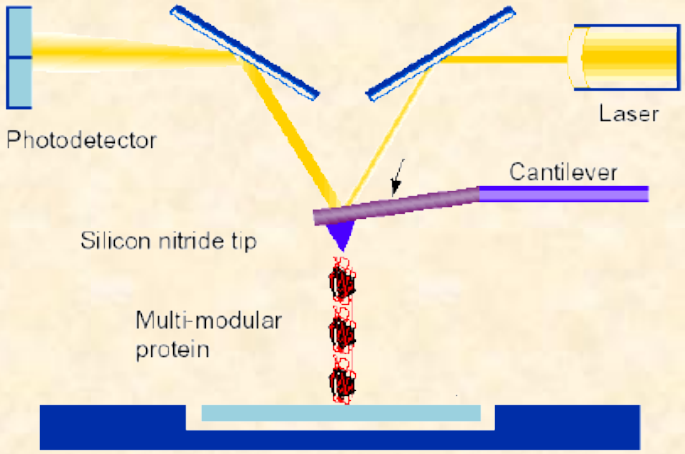


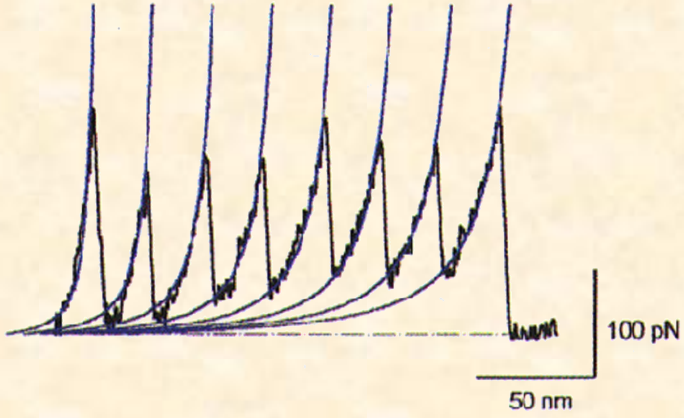
Project Goals

- Develop a Worm-like Chain model for module unwind and fiber fracture
- Simulate module unwind and fiber fracture using a Worm-like Chain model
- Compare results with the experimental response of nacre's biopolymer
- Simulate results with parameter changes to Worm-like Chain model

Worm-like Chain Model

- Mechanical response of a single biopolymer fiber response
- Corresponding experimental response of a single biopolymer
- Unfolding of modules (sawtooth pattern)
- Excellent agreement with the experimental response



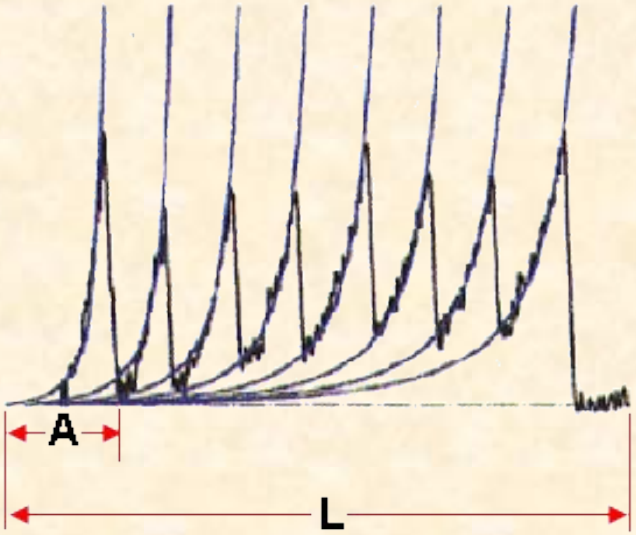


Main Equation of Worm-like Chain Model

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

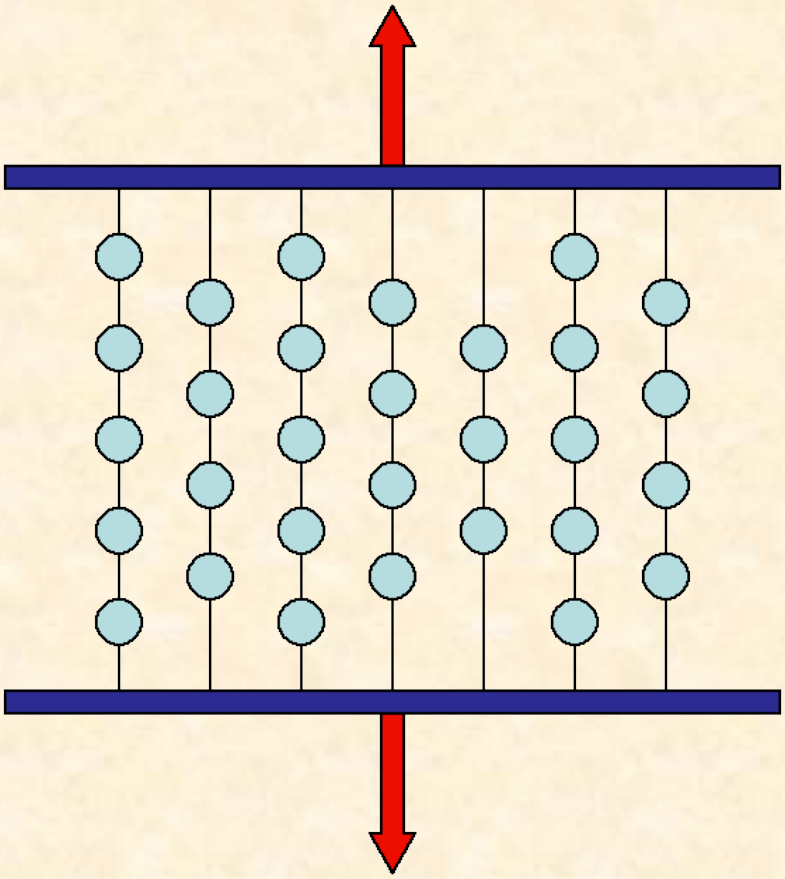
$$f = \left(\frac{k_B T}{A}\right)\left[\frac{1}{4(1 - z/L)^2} - \frac{1}{4} + \frac{z}{L}\right]$$

- k_B: Boltzman Constant
- T: Absolute Temperature
- A: Persistence Length
- L: Contour Length
- z: Extension Length



Fiber Bundle of WLC Fibers with Modular Damage

- Each of the fibers is described by a WLC model
- Random number of modules on each of the fibers which unfolds at random thresholds
- Whenever a module unfolds, the persistence length changes
- Fiber response jumps from one loading curve to another



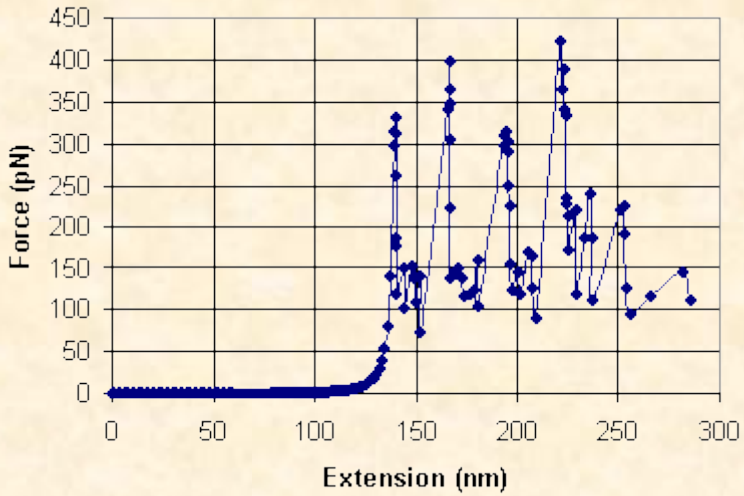
Summary of Research

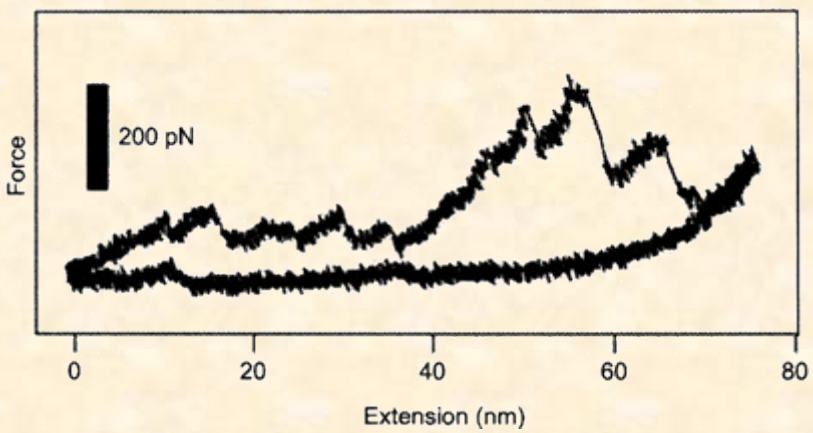
- Learn about experimental response of nacre's biopolymer and Worm-like Chain model of nacre fracture
- Obtain for access to "Cheetah"
- Learn basic Unix commands
- Compile, and run WLC fiber bundle codes on Cheetah

Summary of Research (Continued)

- Use existing WLC fiber bundle code to generate the unfolding events of the modules of protein fibers
- Compare the unfolding events results of the modules of protein fibers with the Force-extension response diagram
- Change parameters of WLC model and simulate results

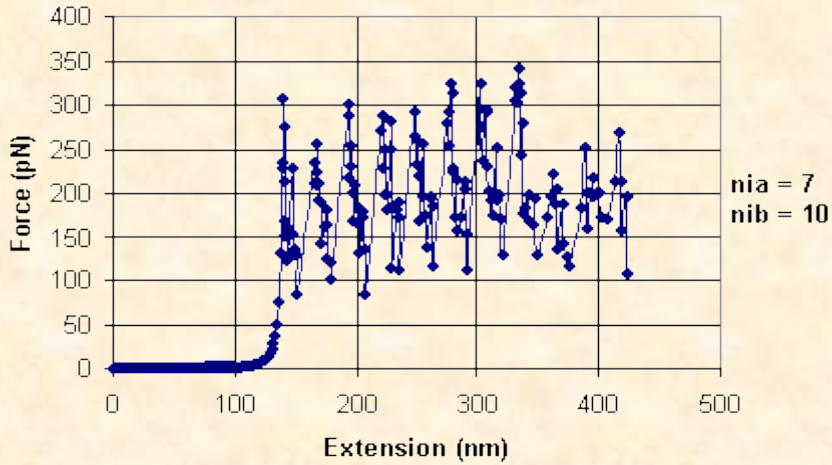
WLC Fiber Bundle Model Results

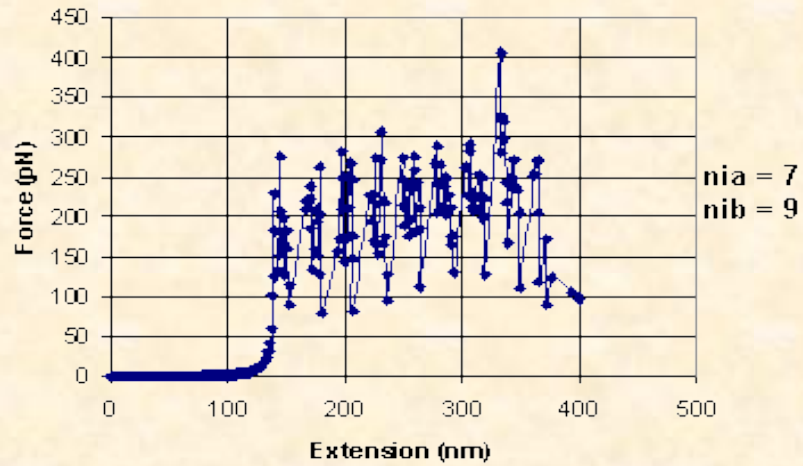


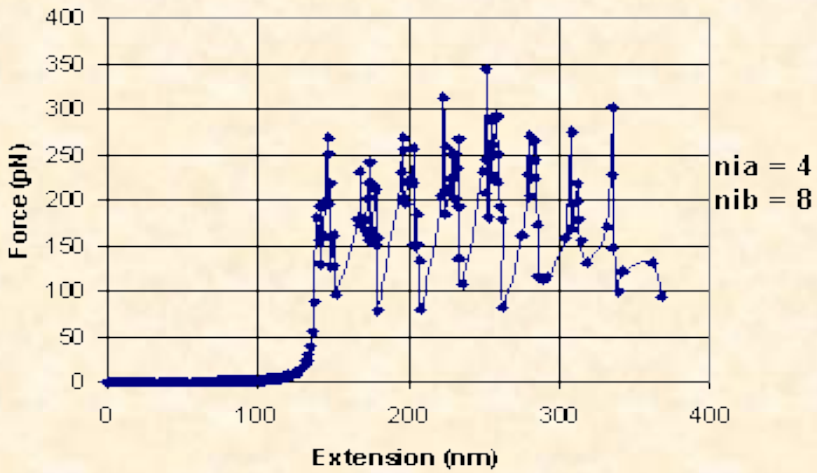


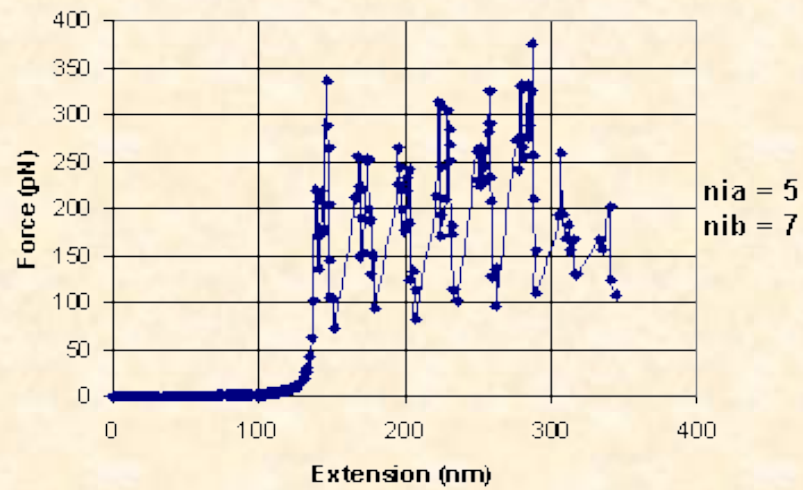
- Generated unfolding events using WLC fiber code
- 15 fibers
- Maximum unfolding force = 420 pN
- Good agreement with the force-extension response diagram

Fiber Bundle Simulation with Modified Number of Modules

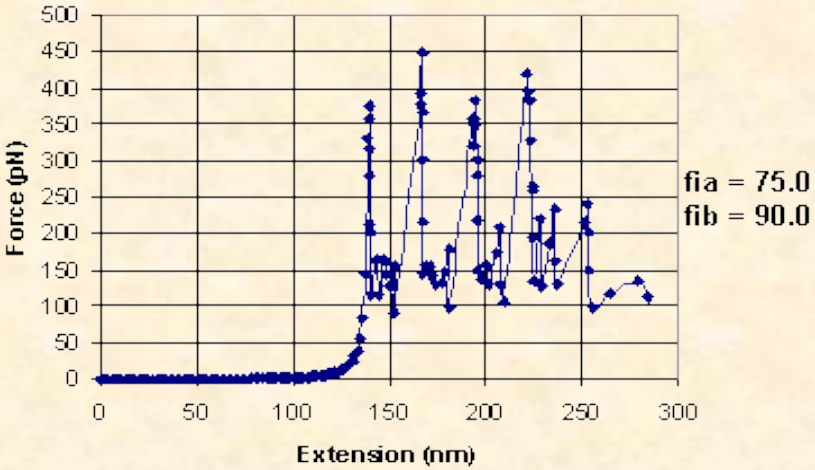


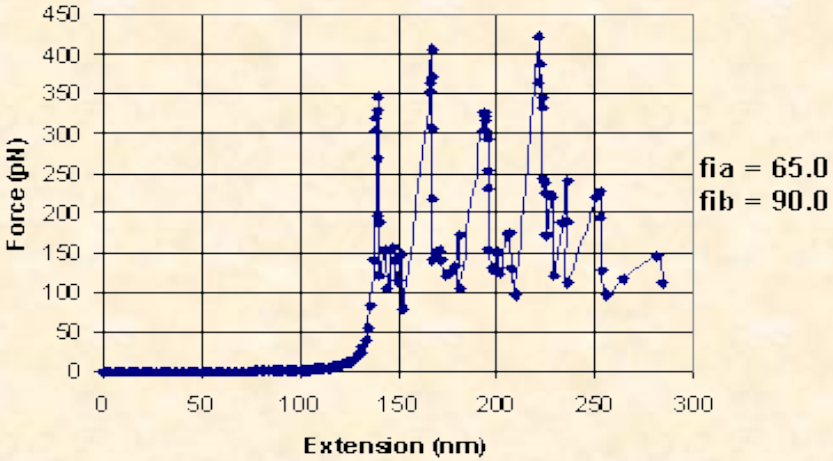


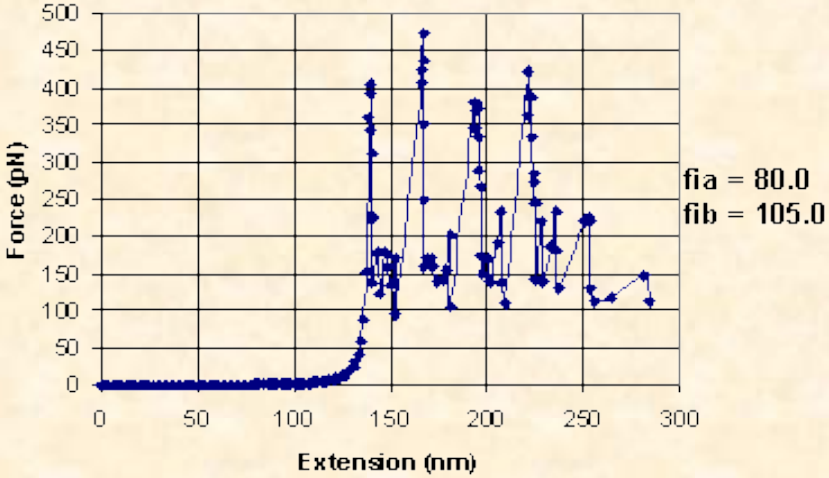


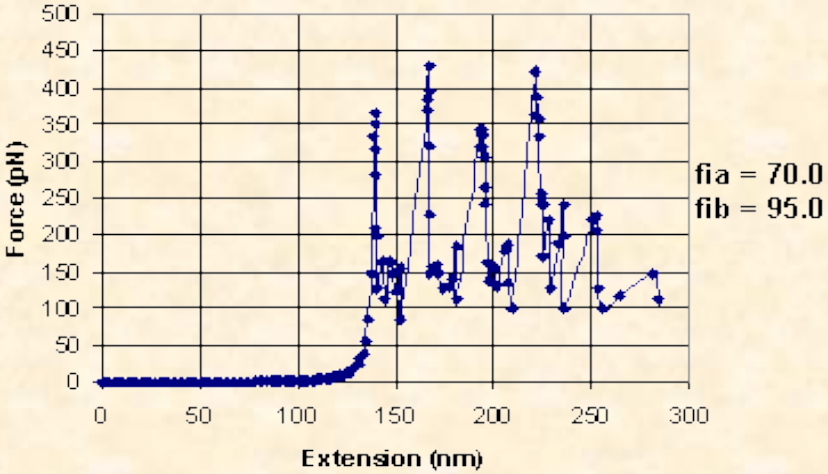


Modified Force Parameters Required to Unwind a Module

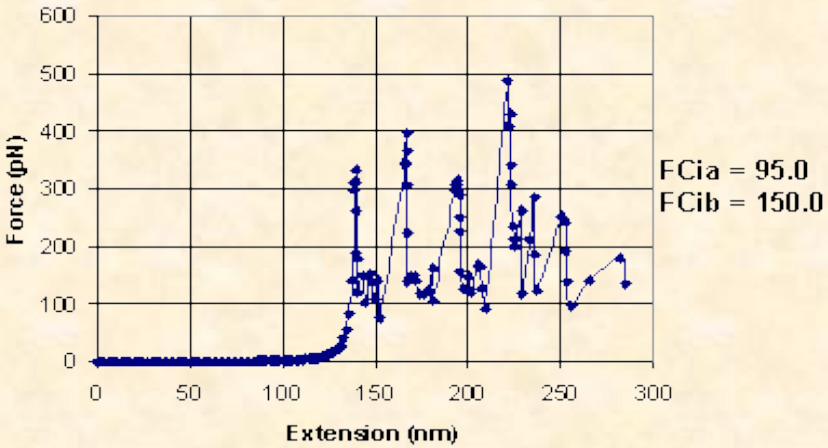


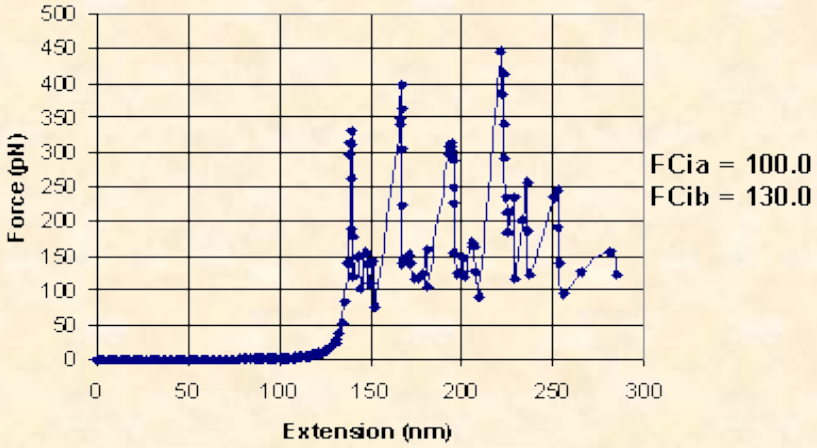


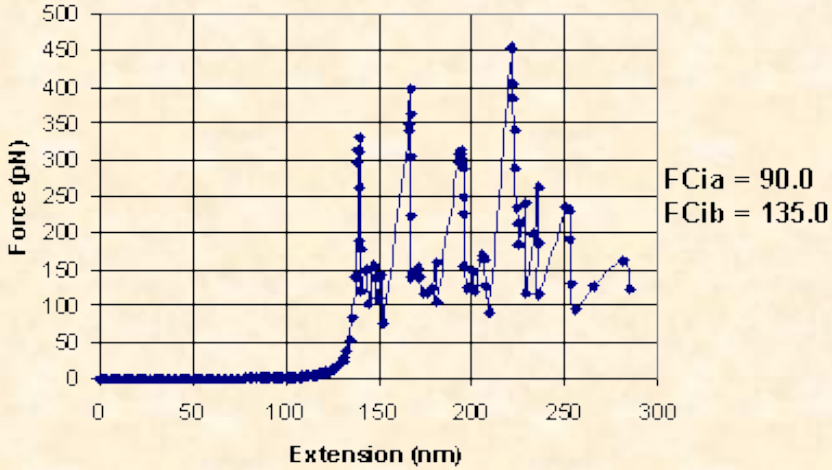


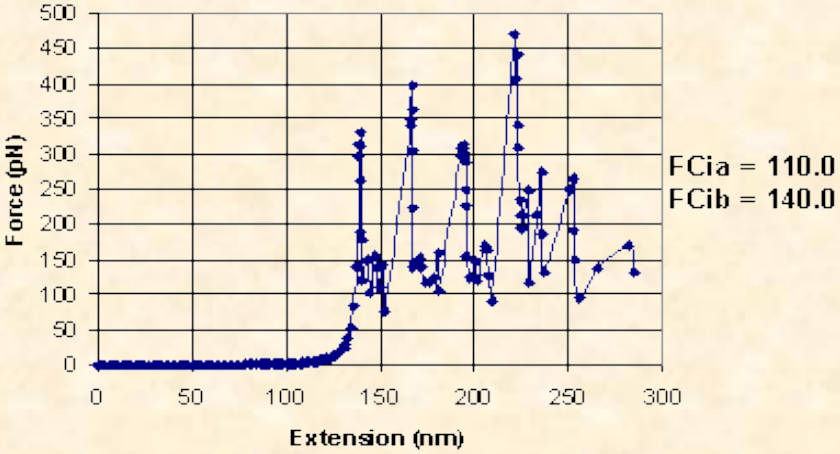


Modified Force Parameters Required to Break the Fibers









Conclusion

- Understand nacre's phenomenal fracture strength and toughness
- Understand experimental response of Nacre's biopolymer
- Better understanding of Worm-like Chain model
- Learned how to simulate unfolding events of the modules using different parameters

Acknowledgements

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Questions?

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