

# Numerical Modeling of Damage Tolerant Biological Material

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## ABSTRACT:

Biomaterialized materials have the ability to employ high volume fraction of modest and brittle materials and still exhibit surprising mechanical performance. Decoding the structure-function relationship of these materials is a challenging task that requires knowledge about the actual loading and environmental conditions of the material in their natural habitat, as well as a complete characterization of their constituents and hierarchical ultrastructure through the use of modern tools such as in-situ electron microscopy, small-scale mechanical testing capabilities, prototyping, and advanced numerical models. In turn, this provides the necessary tools for the design and fabrication of biomimetic materials with remarkable properties. In this work, we will review some of our research activities covering the numerical aspects of fracture and damage in naturally occurring and biomimetic materials, including biomaterialized materials found in hyper-mineralized exoskeleton of mantis shrimps. In our approach, we adopt a finite element methodology that uses a cohesive approach to brittle and quasi-brittle fracture in the mineral.

**Key Words:** Biomaterialized material, biomimetic material, cohesive element.

## INTRODUCTION

*Odontodactylus scyllarus*, known as peacock mantis shrimp, is a common reef associated stomatopod from the tropical Indo Pacific. As described by Patek, et al. [5], the dactyl club of this animal is capable of accelerations up to 10,4g and speeds of 23m/s from a standing start. Moreover, their rapid strike can generate cavitation bubbles between the appendage and their prey, producing, with the collapse of these bubbles, significant stresses at the contact point, in addition to the instantaneous forces upwards of 500N resulting from the direct impact. Despite these significant loads, the dactyl clubs are extremely damage tolerant and are able to withstand thousands of highly energetic blows, a characteristic that, as we describe here, can be directly linked to their ultrastructural features.

## METHODOLOGY AND RESULTS

To gain insights into the damage tolerance of the Dactyl Club Mantis Shrimp and its propodus, we performed dynamic finite element modeling (DFEM) of a striking event against a solid target with the mesh following the complex macroscale geometry of the dactyl and propodus (Figure 2A). To accurately compare the obtained results with previous data from Patek and Caldwell [1] (Figure 1), we modeled the target as a steel cylinder ( $E = 200$  GPa) with 1 mm thickness and 5 mm radius, and based the impact velocity (20 m/s) on their measured final velocity.

We validated the simulations by comparing the computed strike force with the measured one, which gave a comparable value of 550 to 575 N (versus  $693 \pm 174$  N in the experiments). Additional simulations were performed to assess the influence of isotropic damage (cracking) or softening (plasticity) on the stress distribution, with the tensile load to initiate cracking or plasticity ranging from 10 to 50MPa. Although the impact energy absorbed by microcracking or microplasticity reduced the strike force by ~15%, the critical stress values and their overall distribution in the impact region did not change substantially.

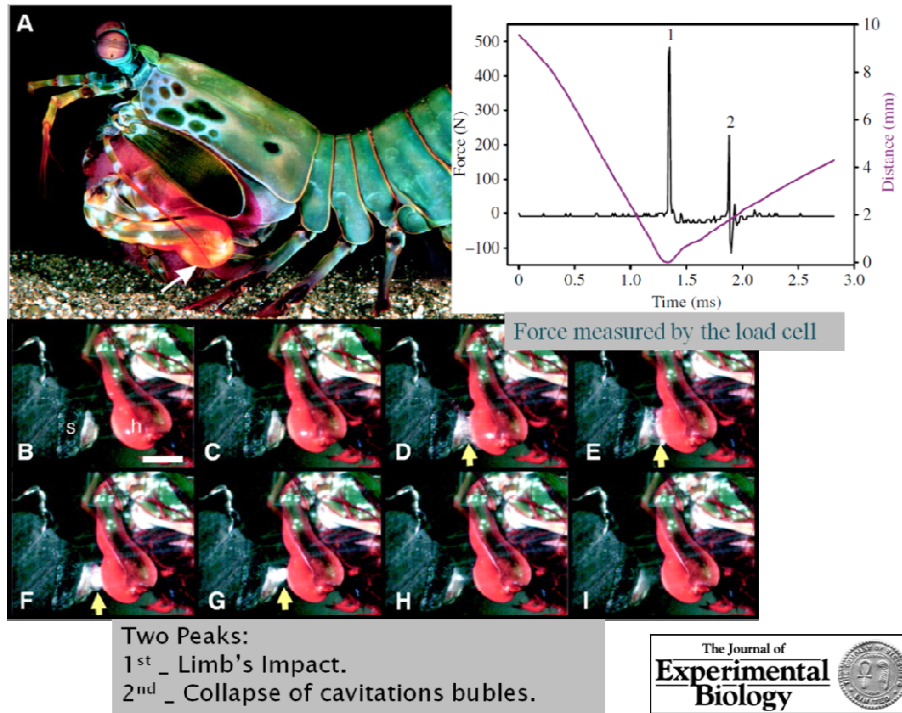


Figure 1- Impact sequence. Data Collected from Patek and Caldwell.

The dynamic evolution of the maximum principal stress ( $\sigma_{\max}$ ) following contact (figure 2B) reveals that the impact wave travels through the entire club and reaches the end of the dactyl  $\sim 2.5$  ms after contact, before being transmitted through the propodus. Because these simulations predict that the maximum values of  $\sigma_{\max}$  are achieved 2 ms after impact, they imply that the propodus has no appreciable effect on the distribution of these critical stress values. Analysis of the maximum stress components at 2 ms after impact (Figure 2C) includes (i) the hydrostatic pressure  $\sigma_H$  (blue tones), (ii) the in-plane maximum principal stress  $\sigma_{IP}$  (iii) the out-of-plane maximum principal stress,  $\sigma_{OP}$  (red tones). These computations imply that the club is subjected to extremely high hydrostatic compressive stresses, with  $\sigma_H$  up to 4GPa reached within a 0.2 mm radius from the contact point. For comparison, the compressive strength of engineering ceramics such as zirconium or silicon carbide is on the order of 2 to 3.5 GPa. Because the dactyl club does not fail catastrophically during impact, this highlights its ability to sustain extremely high levels of localized impact pressure.

DFEM also suggests that internal cracks are likely to nucleate beneath the impact region, the helicoidal architecture (which is located in the periodic region of the dactyl club) (figure 3) provides several toughening mechanisms that hinder catastrophic propagation of such cracks (we will show during the presentation the different microstructure corresponding with each part of the Dactyl and propodus). Charge contrast secondary electron micrographs of coronal cross sections illustrate the tendency of cracks to nest volumetrically within the periodic region between the chitin fibers (figure 3F to H). In three dimensions, this can be represented as a helicoidal fracture pattern propagating between layers, with a rotating crack front that remains parallel to the fibers without severing them. We confirmed this hypothesis by modeling a coronal cross section of a helicoidal stack of fibers curved around a spherical core, which results in the distinctive double spiral-like motif.

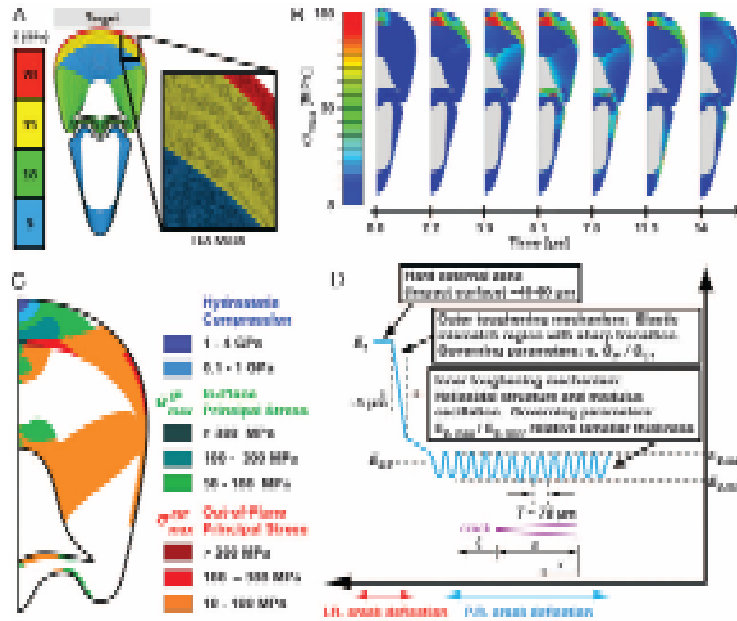


Figure 2- Dynamic finite element analysis (DFEA) and micromechanical modeling. (A) Geometry of the dactyl club/propodus system striking a target at 20 m/s. Color-coding corresponds to the different elastic properties and mass densities used for DFEA simulations (data obtained from nanomechanical characterization of hydrated specimens and synchrotron x-ray transmission studies). (B) Evolution of the maximum principal stress  $s_{max}$  during the impact event until the propagating pressure wave reaches the end of the propodus. (C) Maximal principal stresses within the dactyl club at ~2 ms after impact. (D) Toughening strategies of the dactyl club: (i) hard outer layer for maximum impact force; (ii) modulus transitional domain for crack deflection between the impact surface and the bulk of the impact region; (iii) periodic region with helicoidal pattern and modulus oscillation for crack shielding.  $a$ , crack length;  $x$ , coordinate perpendicular to the crack front propagation;  $x/a$ , relative coordinate ahead of the crack tip in the periodic region ( $x = x - a$ );  $E(x)$ , elastic modulus oscillation.

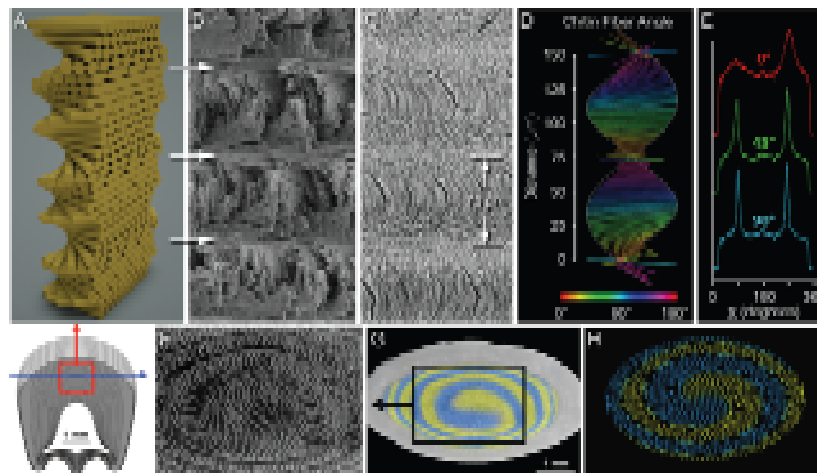


Figure 3- Chitin fibril helicoidal structural motif within the periodic region (with periodicity: ~75  $\mu m$ ). Comparisons between a generalized three dimensional model of a helicoid (A) with an SEM fractograph (B) and a polished surface from a transverse cross section (C). (D) A visualization of the chitin fiber orientations from the x-ray scattering analysis of 92 separate diffractograms obtained through two super layers. (E) Three representative  $c$  plots of the a-chitin (110) reflection used to calculate fiber angles. The plots show changes in  $c$  across the range of angles between each chitin fiber bundle and the x-ray beam. A charge contrast scanning electron micrograph from a damaged coronal cross section (F) with false color (G) and a model of a helicoidal slice (H), which accurately reproduces the fracture patterns.

## CONCLUSION

Our studies show that the stomatopod dactyl club represents a notable departure from previously studied damage-tolerant biological composites, in that it is specifically employed for high-velocity offensive strikes. Our structural investigations, coupled with nanomechanical characterization and finite element simulations, have shown that the club consists of several microstructural features that permit the infliction of crippling impacts while simultaneously minimizing internal damage within the club. These characteristics include a pitch-graded helicoidal architecture constructed from mineralized chitin fibers that can dissipate the energy released by propagating microcracks; an oscillating elastic modulus that provides further shielding against catastrophic crack propagation; a modulus mismatch in the impact region that acts as a crack deflector near the impact surface; and an ultra hard outer layer correlated with a high level of mineralization and a radial organization of apatitic crystallites. The structural lessons gained from the study of this multiphase biological composite could thus provide important design insights into the fabrication of tough ceramic/organic hybrid materials in structural applications where components are subjected to intense repetitive loading.

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