



Multiscale Experiments and Modeling in Biomaterials and Biological Materials, Part I

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Material properties are related to the materials' underlying structures. Biological materials can be defined at the tissue, cellular and molecular levels. Many biological materials have hierarchical structures which range from the molecular scale to the macroscopic scale, which enabled their mechanical properties. They often stimulate the bio-inspired design of engineered materials. In the biomaterials, their macroscopic behaviors are strongly related to their microstructures.

This special topic presents a collection of papers related to biological materials across multiple length scales, including proteins, viruses, eggshells, nutshells, snail shells, celery, enamel, bone, and cardiac tissues. Theoretical, computational, and experimental methods are used to study these materials' structures and their properties from molecular to macroscopic levels. The results provide insights into understanding biological processes, the bio-inspired design of new structural materials and functional materials, and the development of new biomedical materials and devices, including cardiac patches, tissue engineering scaffolds, and implants.

At the time of this writing, it has been about a year since the start of the COVID-19 pandemic. The paper "Differences in interactions within viral replication complexes of SARS-CoV-2 (COVID-19) and SARS-CoV coronaviruses control RNA replication ability" by Katti et al. is timely and insightful.

Jing Du is the JOM advisor for the Biomaterials Committee, part of the TMS Functional Materials Division and Structural Materials Division, and guest editor for the topic "Multiscale Experiments and Modeling in Biomaterials and Biological Materials" in this issue. Dinesh Katti, and Hendrik Heinz are Guest Editors for the Biomaterials Committee.

(Received March 31, 2021; accepted April 1, 2021)

Molecular dynamics simulations were carried out to study the nonbonded molecular interactions among different subunits and domains inside the viral replication complex of two types of coronaviruses, SARS-CoV and SARS-CoV-2. The viral replication complex contains non-structural proteins (nsps). The results suggest that, in contrast to SARS-CoV-nsp12, SARS-CoV-2-nsp12 prefers helices as dominant interacting secondary motifs, indicating the potential relationships between the interaction energies and the RNA replication and transcription rates. Based on this framework, the authors further studied the influence of the drug Remdesivir on the interactions of the SARS-CoV-2 viral complex, pointing to a plausible molecular mechanism of Remdesivir inhibiting SARS-CoV-2, which is by reducing RNA-dependent RNA polymerase (RdRp) and nsp8 interactions.

Healthy teeth in vertebrates are critical for life. The hardest tissue that covers the teeth is the enamel. If compromised, the enamel will not self-repair. Since ameloblasts, the cells responsible for enamel formation, are not present once the tooth erupts in the mouth, natural biological solutions for restoration are not available. The current techniques to repair the enamel involve metallic or polymeric restorations. Amelogenin proteins that regulate mineral deposition during mineral formation have been considered as biological solutions for enamel repair. Snead et al., through their groundbreaking work, have identified a short amelogenin-derived peptide (ADP7) that alone can form a thin layer of enamel to restore essential enamel function. The ADP7 could be used in a clinical environment to restore defective enamel in teeth. Their paper, "Minimal amelogenin domain for enamel formation," provides an in-depth description of the ability of ADP7 to form a thin layer of enamel.

Hierarchy is ubiquitous to biology and plays a vital role in the unique properties exhibited by many materials of biological origin. The paper “Multiscale mechanics of eggshell and shell membrane” by Oyen describes microstructure association to macroscopic fracture resistance of eggshell and shell membrane. The paper illustrates the structure-property relationship of eggs from three sources, hen, ostrich, and alligator, and elucidates the organic shell membrane’s role on the fracture resistance of the eggshells. The study shows that the shell membrane could be a potential target for improving the mechanical properties of eggshell, even if the mineral’s quality is subpar. This work paves the way for using eggshells as biomimetic materials for structural materials applications.

Li and his team contributed a paper titled “In situ observation of fracture behavior of bamboo culm.” *Phyllostachys edulis*, a bamboo species, has long been used as a structural material, because of its outstanding mechanical properties. In this study, bamboo culm’s fracture behaviors were studied using a three-point bending test coupled with an optical microscope, which enabled in situ observation of crack initiation and propagation in its microarchitectures. The fracture behaviors were found to be highly dependent on fiber bundle orientation. Different toughening mechanisms were also discussed for the longitudinal and orthogonal loading conditions. The discoveries can provide guidelines for the future development of bamboo-like composites that can be used as superior structural materials.

The deep-sea snails living near hydrothermal vents exhibited superior resistance to thermal impulse, which is related to their shells’ unique layered structure. In the paper, “Optimal design for higher resistance to thermal impulse: A lesson learned from the shells of deep-sea hydrothermal-vent snails,” Yao and his team investigated the temperature response of a bilayer structure subjected to a thermal impulse on one side. The semi-analytical solutions for the transient temperature field show that the bilayers’ thermal resistance can be optimized by tuning the stacking sequence and thickness fractions of the layers. The results reveal the underlying structure-property relationship in snail shells from deep-sea hydrothermal environments. The results can also provide guidelines for the development of thermal barriers in engineering.

Du and Tan conducted a thorough review of the geometry, microstructure, and mechanical properties for certain edible nuts, almond, brazil nut, chestnut, hazelnut, macadamia, pecan, pistachio, and walnut, in their review article, “Recent studies in mechanical properties of selected hard-shelled seeds: A review.” Ashby charts were generated to compare the geometry and rupture energy of the shells and the kernels in these nuts. The results can be used to improve the processing equipment for

edible nuts. The results can also provide inspiration for the future development of shell-like composite materials and structures.

Naleway, Carlson, and their team contributed a paper titled “Biotemplating of a highly porous cellulose-silica composite from *Apium graveolens* by a low-toxicity sol-gel technique.” Cellulose from Pascal celery was used to fabricate a cellulose-silica composite using a low-toxicity, environmentally friendly, sol-gel technique. The macro-/micro-scale structural features of the fabricated composites exhibited many similarities to celeries. However, the mechanical performances (e.g., elastic modulus and ultimate compressive strength) for the fabricated composites were significantly better than those for the live celeries. This work demonstrated an environmentally friendly processing technique for the fabrication of bio-inspired complex and multiscale composite materials and structures.

Strontium (Sr) is a trace metallic element that exists in natural bones. Strontium ranelate has been shown to promote osteoblast differentiation and new bone formation. In the paper “Fabrication and characterization of Sr-doped hydroxyapatite porous scaffold,” Zhou et al. introduced a novel method of fabricating a three-dimensional Sr-doped hydroxyapatite (HA) porous scaffold. First, preliminary scaffolds were fabricated using an extrusion 3D printing technique that used HA-sodium alginate composite slurry as printing ink. They were then submerged in strontium chloride solutions of different concentrations to control the doping amount of Sr. The results show that the Sr-doped HA scaffold has better compactness and compressive strength than the HA scaffold without Sr doping, and it also promotes cell proliferation and osteoblast differentiation. This work provides an alternative method to fabricate ion-doped ceramic scaffolds for bone tissue engineering applications.

Tan and collaborators have contributed a paper, “The role of recrystallization and local misorientation on the biodegradation behavior of Mg.” The paper describes the influence of recrystallization and local misorientation on the in vitro biodegradation of magnesium at different rolling temperatures. The authors have found that the corrosion rate of the material increased with decreasing rolling temperature. The paper describes the key microstructural factors that affect corrosion resistance, and the differences in the corrosion products created at various rolling temperatures. This work provides an insight into process optimization of Mg-based materials for biomedical applications, where the degradation rate is an important consideration.

In the paper titled “Novel architected material for cardiac patches,” Han, Restrepo, and their team introduced a novel periodic architected material (PAM) with a set of triangular architectures. Using a combination of analytical, computational, and experimental methods, the mechanical behaviors of the PAM were studied. The results show that the

triangular architectures rotated when the PAM was stretched. The effective stiffness and anisotropy of the PAM could be tuned by varying the geometry of the triangular architectures. The PAM shows the potential for fabricating cardiac patches, which is a promising technology to strengthen scar tissue and restore cardiac function after heart diseases.

To read or download any of the papers from this topic, follow the URL <http://link.springer.com/journal/11837/73/6/page/1> to the Table of Contents page for the June 2021 issue (vol. 73, no. 2).

ACKNOWLEDGEMENTS

J.D. acknowledges funding by the National Science Foundation under Grant Numbers CMMI-1826221. D.K. acknowledges funding from National Science Foundation Grant Number OIA- #1946202.

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