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MULTISCALE MECHANICS OF NACRE: FROM MOLECULAR TO MACRO

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ABSTRACT

Nacre, the inner irridescent layer of many molluscan seashells is a biomimetic model for design of next generation nanocomposite systems due to its exceptional mechanical properties. As also true for other biological structural materials, these extraordinary mechanical properties are a result of its hierarchical tracture that covers many length scales. Nacre is composed of three major phases that include inorganic (aragonitic calcium carbonate), organic (proteins), and water. This talk will cover our comprehensive study on mechanics of this multilayer hierarchical biological nanocomposite to evaluate the secret to its mechanics. We have used several experimental (nanoindentation, force microscopy, infrared spectroscopy, macro-testing) as well as several computational and theoretical methods (ab-initio, steered molecular dynamics and finite element modeling). Some of the key results from these studies have been:

(1) Organic exhibits exeptional mechanical properties: elastic modulus of the order of 20 GPa).
(2) Mineral contacts or bridges have minimal effect on mechanics of nacre.
(3) Nanoaspereties have minimal effect on mechanics of nacre.
(4) Viscoelastic behavior of mineral component is observed and the origin of this behavior is attributed to trapped water in mineral, at interfaces and adsorbed water.
(5) Our simulations have indicated that the presence of inorganic phase near the organic phase results in a stiffer response of organic, requiring larger energy during deformation resulting in a contribution to toughness.
(6) Interfacial water and the water ‘bound’ to mineral and water ‘bound’ to protein have significant impact on the organic-inorganic interfacial mechanics.

Time dependent properties of the organic matrix of nacre, as well as its molecular mechanics is evaluated. It was also shown that these responses are dependent on the rate of deformation of organic. Also, we have investigated the specific molecular mechanisms of mineral-organic phase interactions in small and large deformation of

protein at the different rates of deformation. Minerals and proteins form constituents of many biological as well as advanced bioceramic systems and these studies help us understand the biological material systems as well as give key insight into design of next generation biomimetic materials.

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