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Discrete Element Models of Architectured Biological and Bio-inspired Composites

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Discrete element models of architectured biological and bio-inspired composites

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Materials such as nacre and tooth enamel exhibit intricate and ordered microstructures consisting of complex geometrical patterns (e.g., decussating prisms in enamel rods as in Fig. 1, Voronoi tiling in nacre as in Fig. 2). These structures generate specific deformation and fracture mechanisms which lead to outstanding mechanical properties [1, 2]. For example hard, segmented natural structures such as fish or snake scales exhibit similar geometric complexity that ultimately provides puncture resistance and flexibility to a system that is otherwise stiff [3]. Broadly speaking, the unique arrangement of hard and soft phases in natural structures leads to unusual combinations of mechanical properties, a strategy which is now inspiring new types of synthetic materials. Design and optimization tools are however limited, because the mechanics of these materials can be very challenging to capture computationally: The mechanical response of these structures often involves non-linear deformations such as crack twisting in enamel, or large deformation and contact in fish scales or snake scales, which can create convergence issues for traditional solvers. Moreover, large computational models are required to explicitly capture collective mechanisms that may involve hundreds of building elements.

In this work, we present Discrete Element Method (DEM)-based numerical models [4, 5] for three biological materials: enamel, nacre, and scales. The DEM approach relies on the building blocks (enamel rods, nacre micro-tablets, individual scales) being much stiffer than their matrix (proteinaceous interfaces, dermis). With this assumption in hand, the building blocks are modeled as perfectly rigid, and the distribution of tractions across interfaces becomes uniform. DEM models can then capture each individual building block with a single node, while adjacent nodes are connected with nonlinear springs which are governed by the interface properties (elasticity, nonlinear deformations and failure).

In nacreous materials, this approach has allowed us to explicitly simulate the effect of architecture (including statistics) on crack growth, process zone evolution, and the crack resistance curve (Fig. 1b). Similarly, DEM fracture simulations in enamel (Fig. 2b) have quantified for the first time the role of the enamel rod decussation angle on fracture toughness. Lastly, we have combined the DEM approach with the fast contact algorithm of Popov et al [4] to model the bending response of hard scales on a soft membrane, providing unique insights into the flexural compliance as a function of the architecture of the scales skin. The DEM approach can capture the nonlinear deformation and fracture of large volumes (>100,000 building blocks) of complex 2D and 3D architectured materials, so that it becomes possible to explore the interplay between block geometry, arrangement and interface properties in a highly efficient computational manner and at a fraction of the computational cost of finite elements.

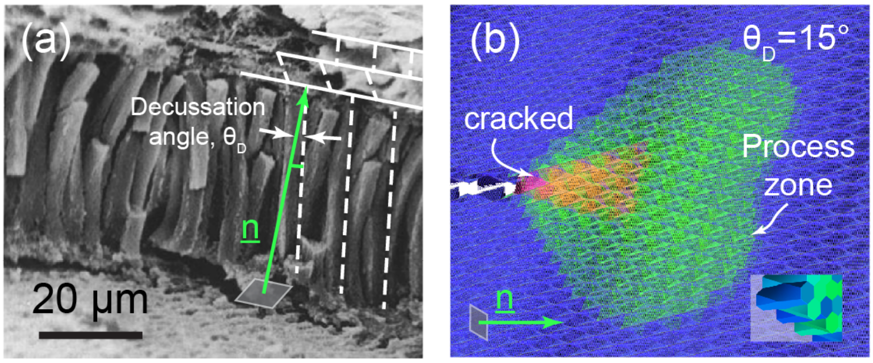

Figure 1: (a) Enamel microstructure showing decussating prism rods [6] and (b) DEM simulation showing crack evolution and process zone growth as load is applied.

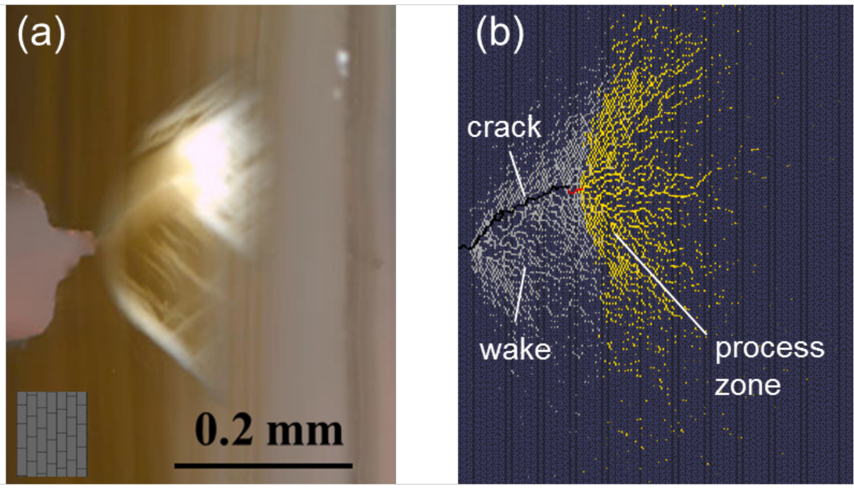

Figure 2: (a) Fracture experiment in pearl oyster nacre [7], where process zone appears as whitened region due to exposed interface ligaments and (b) DEM simulation of fracture capturing crack deflection, process zone toughening and wake in pearl oyster nacre (sheet nacre with statistical variations)

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