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Research paper

Robustness and optimal use of design principles of arthropod exoskeletons studied by ab initio-based multiscale simulations

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ABSTRACT

Recently, we proposed a hierarchical model for the elastic properties of mineralized lobster cuticle using (i) *ab initio* calculations for the chitin properties and (ii) hierarchical homogenization performed in a bottom-up order through all length scales. It has been found that the cuticle possesses nearly extremal, excellent mechanical properties in terms of stiffness that strongly depend on the overall mineral content and the specific microstructure of the mineral–protein matrix. In this study, we investigated how the overall cuticle properties changed when there are significant variations in the properties of the constituents (chitin, amorphous calcium carbonate (ACC), proteins), and the volume fractions of key structural elements such as chitin–protein fibers. It was found that the cuticle performance is very robust with respect to variations in the elastic properties of chitin and fiber proteins at a lower hierarchy level. At higher structural levels, variations of design parameters such as the volume fraction of the chitin–protein fibers have a significant influence on the cuticle performance. Furthermore, we observed that among the possible variations in the cuticle ingredients and volume fractions, the experimental data reflect an optimal use of the structural variations regarding the best possible performance for a given composition due to the smart hierarchical organization of the cuticle design.

1. Introduction and motivation

Most biological materials with structural functions in the animal kingdom consist of an organic matrix of structural biopolymers like collagen and chitin which is modified and reinforced with different proteins and in many cases also with biominerals. The most prominent examples of such materials, like the bones of vertebrates, the exoskeletons of arthropods, and mollusk shells, are known to possess excellent mechanical properties (e.g., in terms of stiffness-to-density ratio and fracture toughness). The origins of these properties have become the subject of intensive research in

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