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Mechanical Simulation of a Diatom Frustule Structure

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Abstract

Diatoms possess intricately complicated nanopatterned silica outer shells, the so called frustules. Due to their excellent three-dimensional (3D) nanostructures, diatom frustules have attracted attentions from many fields to look for potential applications, such as structural material design, light harvesting, photonics, molecular separation and bio-sensing. However, the mechanical property of frustule, especially the role of each single portion that structures a frustule, need to be clearly examined in order to provide a scientific support to frustule utilization. The reported work uses the Finite-Element (FE)-based simulation to investigate the relative mechanical properties of the frustule of the diatom *Coscinodiscus sp.* as compared with reference non-frustule structures. A three-dimensional model for the three featured layers of this frustule and a simplified model for its girdle band are built with the assistance of ABAQUS. A basic-cell concept is suggested; and the comparative results of several simulation groups are reported. The numerical results indicate that the seven-unit-cell model is able to catch the essential mechanics of the *Coscinodiscus sp*. frustule under pressure and that the layered and porous structure of this frustule can effectively resist pressure.

Keywords: diatom frustule, FE, simulation, structure analysis, bio-material

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1 Introduction

Diatoms belong to a major group of algae. They are among the most common phytoplanktons living in almost every aquatic environment on the earth. One of their extraordinary capabilities is to absorb soluble silicon from water and then process the silicon into a highly complicated, pored silica cell wall, called as the frustule[1]. Some species may have multiple layers of silica in their frustules. Generally, a frustule consists of two joined valves, termed as the hypovalve and the epivalve, respectively. Sometimes, they are called as the inner and outer valves since the outer valve is slightly larger, allowing the inner valve to fit inside and form a certain sealed overlap around the frustule equator. Each of these two valves contains either one single layer or multiple layers of silica that binds together to form a void chamber. A band of silica, called as the girdle band, wraps around the diatom equator and holds the epivalve and hypovalve together[2]. Most types of diatoms have their own specific patterns of hole arrays, called as areola, in their frustules.

Diatom frustule is composed of biosilica, which has been considered as a composite material since about 40 years ago. It is mainly composed of amorphous hydrated silica $S_iO_2{\cdot}2H_2O$[3] with a small proportion of organic macromolecules, which is believed to control both the silica deposition and the nanopatterning process[4]. Reimann *et al.* used the vapor of hydrofluoric acid to remove the silica and then revealed the organic material[5]. Every part of the silica shell of *Cylindrotheca fusiformis* was tightly surrounded by organic material, and the whole cell wall was surrounded by a mucilaginous substance. Three families of cell wall proteins (termed as frustulins, pleuralins and silaffins) and extremely long-chain polyamines of *Cylindrotheca fusiformis* were discovered[6–9]. These long-chain polyamines were attached to the polypeptides, noted as silaffins[10] that were able to precipitate silica within seconds during the formation of biosilica, termed as Silica Deposition Vesicles (SDVs). Types of silaffins and how they affect the silica formation are still under research.

The diatom frustule possesses several intriguing

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mechanical properties. Living in a natural environment, diatoms are exposed to survival challenges like predation, collision and impact by particles flowing in the water. Thus, frustule must be strong enough to face those challenges. From the perspective of the theory of evolution, mechanical protection of the diatom frustule should be acquired by using both minimum material and energy consumption to maximize its strength. Hamm *et al.* explored the defense potential of a frustule as a passive armor against predators by matching the data from an experiment with the results from a finite element simulation[11]. In this research, an inverse relationship between frustule size and mechanical strength was revealed, where the mechanical stresses ranged from 150 MPa to 680 MPa. In another paper, Hamm explained the relationship between mechanical challenges and the structural components[12]. In his simulation, a compressive force (about 0.75 mN) was acquired through a micro-needle pressing test and the force was applied on diatom *F. kerguelensis* to simulate an imaginary mandible bite from the predator. Before reaching the breaking limit of the girdle band, exceptional high compressive stress was obtained during the simulation. He then concluded that the frustule indicated an evolutionary optimization in response to this high stress. Different from the micro-needle-technique used by Hamm, the Atomic Force Microscope (AFM) was employed by researchers to investigate the basic mechanical parameters. Almqvist *et al.* studied the silica shell of diatom *Navicula pelliculosa*[13]. The delicate structures were imaged and the micromechanical properties were measured. The elastic modulus was found to vary from 7 GPa to hundreds of GPa depending on locations, and the hardness ranged from 1 GPa to 12 GPa. Subhash *et al.* presented the nanoindentation result of the frustule of diatom *Coscinodiscus concinnus*[14], showing that the porous diatom frustule exhibited a low Young's modulus of about 0.591 GPa to 2.768 GPa in the central area and 0.347 GPa to 2.446 GPa at locations far away from the center, suggesting that the frustule was not homogeneous. Losic *et al.* investigated the hardness and elastic modulus of *Coscinodiscus sp.* diatoms using an AFM-based nanoindentation[15]. Significant differences were observed in three layers, in which the modulus ranged from 1.7 GPa to 15.61 GPa and the hardness from 0.076 GPa to 0.53 GPa. Nanoindentation loading and unloading curves were acquired at different locations, indicating that the frustule was not homogeneous. Note that all these measurements were conducted on frustules, likely to be the properties of the localized structures, rather than the material itself. Such localized experiments cannot reveal a big picture of the diatom frustule, especially considering both the material and the featured structure.

Due to their interesting three-dimensional nanostructure, diatom frustules have drawn attentions from many applications like light focusing[16] and manipulation[17], photonics[18], molecular separation[19], biosensing[20,21] and drug delivery[22]. Diatom frustules as a structured material will attract growing attentions despite of many questions unanswered.

The work reported in this paper intends to explore the basic structures that construct a frustule and to understand the mechanical properties of such structure of the diatom *Coscinodiscus sp.* via 3D ABAQUS Finite-Element (FE) modeling and simulations. The mechanical features of the frustule are investigated through comparisons with reference structures without the diatom holes. In addition, the girdle band is also modeled and comparative simulations are conducted. It should be pointed out that the diatom frustule exhibits an obviously brittle failure[11]. Thus, applications of the diatom material, or structure, should be confined in its elastic regime and so is the main target of the current work. Other issues, such as buckling and crack initiation/propagation should play a role in the final failure process and they needs further study to complete the whole story.

2 Simulation models

The frustule of the *Coscinodiscus sp.* diatom appears like a short cylindrical box with a top dome. The observation of its structure reveals that the external surface of this frustule consists of repeated hole groups of similar size. Thus, it is reasonable to assume that there is a smallest and repeatable basic structure as the unit cell of the frustule. Then, an FE model can be created by assembling such unit cells up. Simultaneously, solid structures of the same material volume are created as the references to explain why diatom chooses to form frustule instead of a simple solid structure. Two key parameters, the maximum von Mises stress and the maximum displacement are used as the indicators to evaluate the structural characteristics of the frustule.