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Development of a new NanoHUB Simulation Tool: Coarse graining of Crystalline Nano-Cellulose.

Kuo Tian, Mehdi Shishehbor, and Pablo Zavattieri
Department of Civil Engineering, Purdue University

ABSTRACT

Crystalline Nano-cellulose (CNC) is a general molecular structure obtained from acid hydrolysis of native fiber. They are often very short (100 to 1000 manometers) and the mechanical properties of CNC varies depend on length scale. Due to defect formation of the structure, the mechanical properties of the material composed of such CNC may vary drastically. This study was to provide a numerical tool to integrate a few valid modules and to better understand the mechanical properties of CNC and the overall performance of the bio-inspired material composed of CNC. Our focus is mainly on two type of composite structure [1] bouligand structure which is found in mantis shrimp and [2] staggered structure based on bone structure. The Mechanical test on these structures can provide useful information on their type of failure and the effect of length and arrangement of CNC on overall mechanical properties. The tool was built with the instructions from nanohub using Rappture as GUI designer and Python as programming language. The key method is to generate the structure file using base structure of CNC and user input, then send shell command to computation and visualization package. Advanced data structures were used to ensure when duplicating in length formation of the cellulose doesn't change. The results were almost the same with previous data obtain from a rather slow simulation. The simulation was 20% faster since the study optimized on structure generation. The computational package was external and it was where most of the time consumed. The overall performance of tool was sufficient to help fellow researchers and students to get a quick and accuracy mechanical property of a chosen CNC structure.

KEYWORDS

Crystalline Nano-cellulose, bouligand, nanohub, Rappture