8th. World Congress on Computational Mechanics (WCCM8)
5th. European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008)
June 30 – July 5, 2008
Venice, Italy

Understanding Mechanical Behavior of Protein Crystal Using Coarse-Grain Model

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Key Words: *Protein, micromechanical model, Tensile loading, Coarse-Grain Model*

ABSTRACT

Proteins have been known to perform the excellent mechanical functions and exhibit the remarkable mechanical properties such as high fracture toughness in spider silk protein. The spider silk protein has high fracture toughness ~1GPa comparable to steel [1]. The fact displays that the mechanical characterization of protein molecules and/or crystals is very essential to understand such remarkable mechanical function of protein molecules. In this work, for gaining insight into mechanical behavior of protein crystals, we developed the micromechanical model by using the empirical potential field prescribed to alpha carbon atoms of a protein crystal in a unit cell (coarse-graind model) rather than by using the full atomic model with taking up to 26 hour in PC. The basic structure of proteins, helical and sheet structure, have been used in this study (Fig. 1). We could get their mechanical behavior under tensile loading. We also confirmed that the protein has the tendency of elastic-plastic material [2], and obtained the same modulus of elasticity of the protein with proposed model as the one using full atomic model. From the previous works, we may obtain a strength of α-helix and β-sheet. Furthermore, we may observe the proteins' behavior when they are applied another type of force.

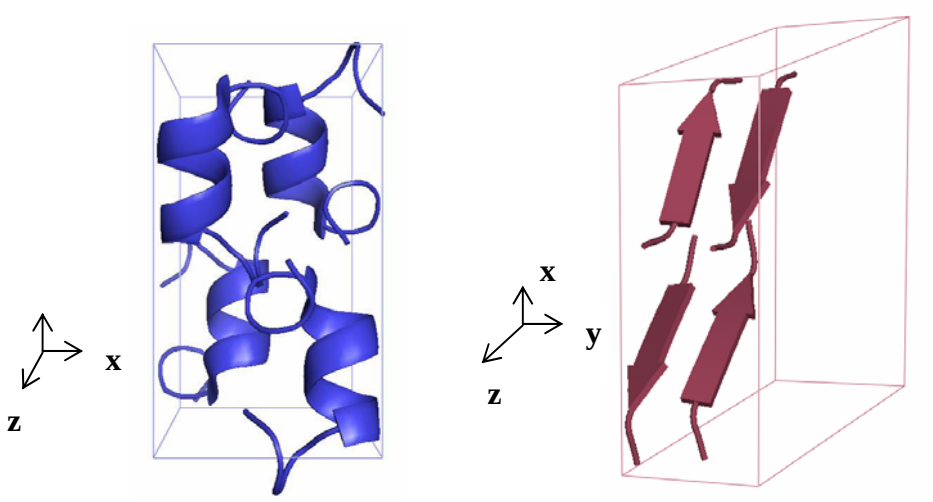

Fig. 1 A cartoon of a unitcell of α-helix (left) and β-sheet (right)

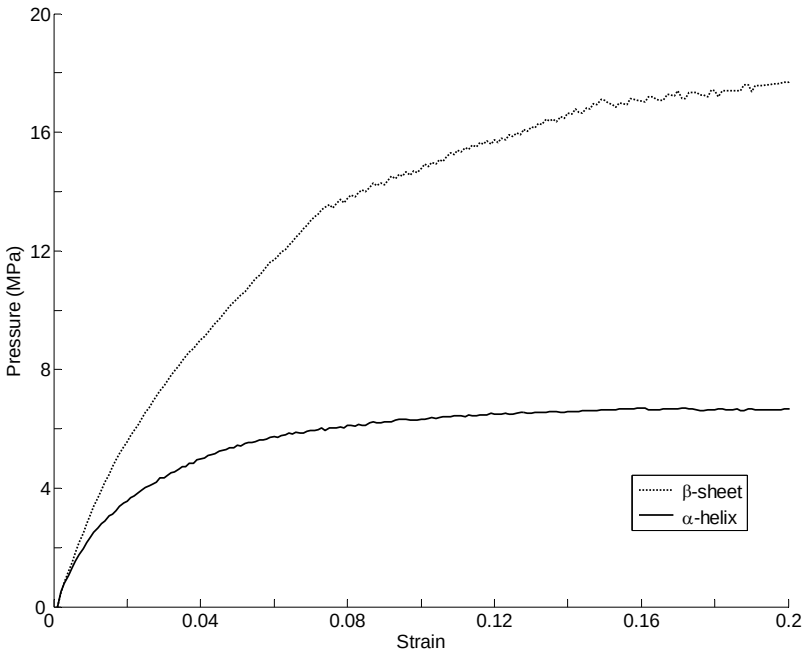

Fig. 2 Pressure-strain curve of α-helix and β-sheet

ACKNOWLEDGEMENT

This work was supported in part by KOSEF (Grant No. R01-2007-000-10497-0), MOST (Grant No. R11-2007-028-00000-0), and BK21 Project (to S.N.). The authors declare that there is no conflict of interest.

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