11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
July 20 - 25, 2014, Barcelona, Spain

A Molecular Dynamics Study on Mechanical Properties of *Bombyx mori* Silk Fibroin

Yuan Cheng[1]*, and Yong-Wei Zhang[1]

[1] Institute of High Performance Computing, A*STAR, Singapore 138632
Email: chengy@ihpc.a-star.edu.sg

Key Words: *Silk fibroin, Molecular dynamics simulation, Water effect, Mechanical property.*

Silk fibroin has attracted great attention due to its superior mechanical properties such as ultra-high strength and stretchability, biocompatibility, as well as its versatile biodegradability and processability. Although its strength is well-known to be controlled by the dissociation of protein chains from β-sheet crystallite, the way that water as the solvent affects its strength and the reason that its theoretically predicted strength is several times higher than experimental measurement remain unclear [1]. In this study, we perform all-atom molecular dynamics simulations on β-sheet crystallite of *Bombyx mori* silk by pulling out β-chains at different locations from the crystallite with/without water solvent. The crystallite unit structure and the snapshots for pulling out the targeted chains are illustrated in Figure 1.

Hydrogen bond formation and strength are important in determining the stability and the failure strength of the crystallite. We examine the different behavior of hydrogen bonds in vacuum and in water by carrying out long time equilibrium molecular dynamics simulation. It was found that compared to the vacuum environment, both the number and lifetime [2] of the hydrogen bonds between β-chains in water are reduced, and thus greatly weakens the strength of silk fibroin.

We also find that the ultimate tensile force for pulling out a β-chain from a crystallite unit is strongly chain-location-dependent. As shown in Figure 1., the pulling strength for the interior chains is several times higher than that for the surface/corner chains, from which we identify the weakest link that dictates the failure process. Hence, the present work sheds light on the role of water in the strength of silk fibroin and also provides clues on the origin of the strength difference between theory and experiment.

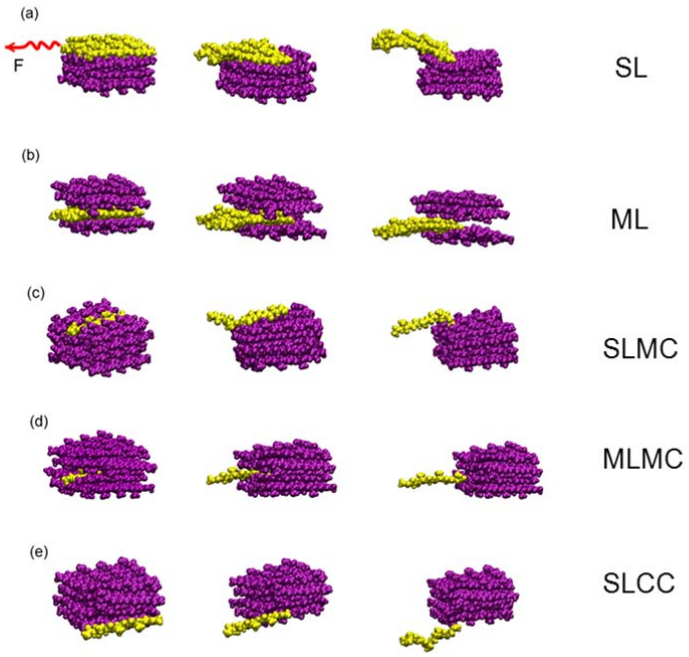

Figure 1. Representative snapshots for pulling out the β-chains from different locations of the crystallite unit. (a) Surface layer (SL), (b) (middle layer) ML, (c) surface layer-middle chain (SLMC), (d) (middle layer-middle chain) MLMC, and (e) surface layer-corner chain (SLCC). The chains being pulled out are displayed in yellow, while the rest are displayed in purple.

REFERENCES

[1] Keten, S., Xu, Z., Ihle, B., & Buehler, M. J. 2010 Nanoconfinement controls stiffness, strength and mechanical toughness of beta-sheet crystals in silk. *Nat Mater.* **9**, 359-367.

[2] Luzar A. & Chandler. D. 1996 Hydrogen-bond kinetics in liquid water. *Nature*, **379**, 55-57.