Mechanical Properties of Silk Fibroin and Silk-Graphene Interactions based on Molecular Simulations

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As a widely available biomaterial with good thermal and optical properties, silk fibroin is a natural protein fiber possessing an excellent mechanical strength. It has attracted great attention due to its outstanding mechanical and physical properties such as ultra-high strength and stretchability, biocompatibility, as well as its versatile biodegradability and processability.[1,2] They can be made into various morphologies such as sponges, hydrogels, films, mats and particles, facilitate their wide applications as apparel/medical textiles, surgical sutures, drug/gene carriers, tissue engineering scaffolds, sensors, etc. Great efforts are demanded in order to further enhance the mechanical properties of silk fibroin. In this study, large scale molecular dynamics simulations were carried out on interactions between graphene substrate and model peptides with different sizes extracted from different domains of silk fibroin. The simulation result on secondary structure component of peptides agrees well with the experimental data. Our study shows that graphene substrate has different impact on structural properties of different domains of silk fibroin.[3] Mechanical tests were also carried out on representative peptides to measure the mechanical properties of the peptides related to strength and resilience. It was shown that the stregnth of the peptides are enhanced upon adsorption to the graphene surface. Our results provide insightful understandings in structure-mechanical property correlation of silk protein upon adsorption to the substrate, and will helpful to future design of bio-inspired composite materials, especially in biomedical application areas.

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

References

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