ABSTRACT

Silk Fibroin-hydroxyapatite (SF-HAP) bio-nanocomposite is a prospective biomaterial for tissue engineered graft or scaffold for bone repair. Here, SF is primarily a soft, organic phase and HAP is a stiffer, mineral phase. Silk fibers, majorly produced by silkworms (e.g. *Bombyx mori*), is a promising biopolymer for use in biomedical applications such as tissue engineered grafts as it is a load bearing biopolymer with biocompatible and bioresorbable properties. *Bombyx mori* Silk Fibroin (*B. mori* SF) is a hierarchical bio-macro-molecule made up of amino acid residues consisting of crystalline phase and amorphous phases. Understanding about the mechanical behavior of *B. mori* SF at multiple length scales is of importance when developing tissue grafts, which requires a deeper understanding of deformation behavior and involved molecular mechanisms at nanoscale. Along with the mechanical behavior of *B. mori* SF, the interfacial interaction between SF and HAP also, is a defining factor for the mechanical performance of SF-HAP bio-nanocomposite. To investigate such nanoscale behavior, molecular dynamics method is a preferred approach. This study focuses on understanding of the mechanical properties and deformation mechanism of *B. mori* SF at nanometer length scale, considering the effect of structural aspects and chemical environment. For this purpose, phenomenological atomistic models of *B. mori* SF nanostructures are developed, based on connectivity and relative arrangement of crystalline and amorphous domains. Tensile loading based mechanical behavior analysis of these *B. mori* SF models were performed using Molecular Dynamics (MD) simulations and compared with existing results from literature. Elastic modulus of ~7.4GPa and tensile strength of ~340 MPa were obtained for this model. Analysis of results reveals that deformation mechanisms in *B. mori* SF at nanoscale are a combination of tensile and shear deformations, wherein, the tensile deformation of amorphous region results into excessive

extension of *B. mori* SF, whereas, shear deformation of crystalline region results into a high tensile strength. Moreover, current study also focuses on the role of interfacial interaction between SF and HAP in overall mechanical behavior of SF-HAP bio-nanocomposite. For this purpose, SF-HAP interface models based on HAP crystal size and HAP surface in contact with SF has been developed. Pull-out tests are performed to analyze the interface debonding behavior of these SF-HAP interface models using Steered Molecular Dynamics (SMD) simulations. Current work contributes in developing an understanding of mechanistic interactions between amorphous and crystalline domains in *B. mori* SF nanostructure and between the protein and mineral phases in SF-HAP bio-nanocomposite.