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MECHANICS AT THE MOLECULAR SCALE IN BONE

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ABSTRACT

Bone is the primary structural component of the human body. It supports the body structure and performs diverse functions like production of white and red blood cells, various ions for bodily functions etc. The primary constituents of bone are the mineral hydroxyapatite (HAP), the protein: collagen, and water. The collagen molecule is triple helix with three polypeptide chains. Each chain has 1014 residues with GLY-X-Y repeating units where X-Y are proline-proline or hydroxyproline-proline respectively. Also, the ends of helical collagen molecules are non-helical. These non-helical regions are known as 'Telopeptides'. The dimensions of mineralized HAP nanocrystals are 50 nm × 25 nm × 3 nm. In bone, HAP provides the toughness and rigidity whereas collagen molecules provide the tensile strength and flexibility to bone. As also observed in several structural biological materials such as teeth, and seashells, the unique mechanical properties of bone are a result of its structural hierarchy, or order over several orders of length scale. The microstructure of bone consists of cylindrical motifs which are known as osteons. These osteons have concentric lamella structure. Lamella is formed from collagen fibers which consist of collagen fibril. At the collagen fibril, HAP mineralizes at specific locations known as 'hole zones'. The typical size of the 'hole zone' is about 20 nm. The collagen molecules interact with these HAP nanocrystals in a specific orientation where c-axis of HAP aligns parallel to collagen chains indicating that the (0001) surface of HAP interacts with the collagen molecule. Thus, collagen interacts with (0001) surface of HAP through telopeptides.

Here, we have used molecular Dynamics (MD) and Steered MD (SMD) simulations to simulate a composite system consisting of inorganic (HAP) and organic (collagen) phases using CHARMm force field. The mechanical behavior of molecular collagen in natural bone have been assessed by pulling the collagen molecule in close proximity and in absence of HAP. The pulling has been performed in both parallel and transverse directions. All the simulations have been performed by using NAMD [1]. All the models are first geometrically optimized through energy minimization before performing MD and SMD simulations. During, SMD simulations, force is applied to selected atom/atoms.

The load-deformation behavior of collagen in absence of HAP shows distinct differences from the load-deformation behavior of collagen in close proximity of HAP. It is observed that with breaking of hydrogen bonds, water molecules get incorporated within the collagen chains. The nature of this incorporation is different in collagen in absence of HAP as compared to the collagen in close proximity of HAP. We have therefore shown that the proximity of HAP significantly influences the interaction between collagen and water and thus the mechanics of bone.

In addition, we will also decribe our experimental studies on quasistatic and dynamic nanomechanical behavior of bovine bone. Our studies evaluate the origin of viscoelastic behavior and the role of heterogenieity and microstructure.

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