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TITLE

Nanomechanics of tropocollagen and hydroxyapatite biomaterials with an account of collagen mutations and varied hydroxyapatite textures: Implications for bioinspiration, disease mechanics, and material mechanics

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Hierarchical nanocomposite materials such as bone, dentine, nacre etc. are primarily composed of organic (polymeric polypeptide Tropocollagen (TC) chains) and inorganic (calcium hydroxyapatite (HAP) and calcium carbonate) phases. Interfacial interactions between the organic phase and the mineral phase as well as the structural effects arising due to the staggered arrangement, TC mutations, and varied HAP textures significantly affect the strength of such biomaterials. In addition, the above factors also influence the pathology of a biological tissue. The effect of such factors is intricately intertwined with the chemical environment of such materials. In the present investigation, different idealizations of TC-HAP composite biomaterial system under tensile and compressive loadings are analyzed using explicit three dimensional (3-D) molecular dynamics (MD) simulations to develop an understanding of these factors. The analyses focus on understanding the correlations among factors such as the structural arrangement, the peak stress during deformation, the Young's modulus, the peak interfacial strength, and the length scale of the localization of peak stress during deformation. Analyses show that maximizing the contact area between the TC and HAP phases result in higher interfacial strength as well as higher fracture strength. Due to the staggered arrangement, the orientation of HAP crystals has insignificant effect on the biomaterial strength in comparison the effect observed when a series of HAP-TC interfaces could be formed in parallel. Analyses based on strength scaling as a function of structural hierarchy reveal that while peak strength follows a multiscaling relation, the fracture strength does not. The peak strain for failure was found to be independent of the level of structural hierarchy. Analyses include effect of collagen mutation to different types of residues as well as genetically affected variations. Analyses are extended into quantum mechanical domain to elucidate role of electronic contributions. Results are discussed in terms of possibility of motivating bio-inspired materials and well as to explore possible disease mechanics issues.