Molecular dynamics to study interaction and mechanics in composite bone biomaterials

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Abstract

Composite biomaterials of polymers and minerals are widely investigated for total bone replacement. The molecular phenomenon at interfaces between polymer and mineral is known to have significant contribution on overall mechanical properties of the composite systems. Often molecular dynamics (MD) simulations are used to analyze interactions at interfaces. MD simulations use a potential function (forcefield) to calculate different thermodynamic properties and structural behavior of the structures. Parameters of these forcefields are generally obtained from different experimental methods or by rigorous quantum mechanical calculations. We have modeled interfaces between hydroxyapatite (mineral) and polyacrylic acid (polymer). For hydroxyapatite (HAP), parameters were obtained in CVFF forcefield. These parameters were validated by comparing the computationally obtained unit cell parameters, vibrational spectra with XRD and FTIR experiments. Interaction study was performed between HAP and polyacrylic acid (PAAc) with obtained parameters of HAP and available parameters of PAAc. The simulations indicated that the HAP mineralization in the presence of PAAC is a biomimetic process where polymer chains are aligned parallel to c-axis of HAP. Different types of chelating structures were formed at interfaces of composites. Hydrogen bonds were also observed involving surface atoms of HAP and carboxylate groups of PAAc. Also, steered molecular dynamics (SMD) simulations were performed at constant velocity. Here, PAAc was pulled in presence and absence of mineral to understand the change in mechanics of polymer due to the non-bonded interactions with mineral. This study shows that the unbinding potential of polymer is different in absence and in presence of mineral, which indicates that the mechanical properties of polymer have significantly impacted by the presence of mineral.