Mineral influences the mechanical behavior of protein in natural nano biocomposite nacre

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Abstract

The natural biocomposite nacre has 95-98% of aragonite, which is a polymorph of calcium carbonate and the rest organics mainly in the form proteins. In spite of having such high aragonite content this biocomposite shows fracture toughness which is three orders of magnitude higher than geological aragonite. The presence of this small fraction of organic thus brings a considerable alteration in its mechanical properties. The organic is found to be wrapped around the aragonite platelets giving rise to familiar brick and mortar structure. The contribution to this enhancement of property could result from two different length scales. One, the micro structural effects in the length scale of 10^{-6} m, and the other, from the atomic level or the nano scale length of 10^{-9} m. In this work we deal with the phenomenon related to second scale. In our previous work while investigating the cause of this improved mechanical properties we observed that the organic present shows a high elastic modulus of about 15-20 GPa, which is significantly higher than any other bulk protein. This organic is also found to have an ability to undergo large deformation. In this work we focus on determining how the presence of mineral aragonite influences the mechanical behavior of protein and causes it to behave different from other existing proteins. Molecular Dynamics simulation has been used to conduct this study. It is observed that the work required to unfold a certain domain of a protein in presence of aragonite is approximately five times more than work required to be done in absence of it for the same amount of displacement. This work provides an insight into how aragonite influences the motion of the atoms in the protein and thus affects the stiffness of different portions of the protein.

Keywords: Protein unfolding, Molecular Dynamics, nacre.