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Nanomechanical properties of polymorphic amyloid nanowire using molecular dynamics simulation

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The hIAPP (human islet amyloid polypeptide) causes the Type II diabetes which known as the degenerative diseases.[1] These hIAPP exists at fibril shape which disrupt the normal insulin secretion in beta cell of pancreas and not easily decomposed at physiological conditions. Also hIAPP have polymorphic characteristic which has different shapes and properties. So, finding the mechanical properties of hIAPP fibril is crucial for understanding the type II diabetes.

Several measurements used for the detection and characterization of protein materials such as SEM (Scanning Electron Microscopy), TEM (Transmission Electron Microscopy), AFM (Atomic Force microscopy) and optical tweezer. Most of all, force spectroscopy such as AFM and Optical tweezer has been used to reveal the biological behavior of functional proteins and to characterize the mechanical properties of proteins. However, these force spectroscopy has difficulty in analyzing polymorphic structure of amyloid structure and measuring the mechanical properties of nanoscale amyloid fiber. To overcome the limitation of force spectroscopy, simulation is one of the efficient methodologies to probe the mechanical behavior at atomic resolution. Among several provided methods, MD (Molecular Dynamics) is a useful tool to describe the mechanical properties of amyloid fibrils in detail.

In this study, the polymorphic structures of hIAPP, parallel homo (Pho) and parallel hetero (Phe) structures are constructed by molecular modeling and equilibration process with MD program ‘NAMD’. Subsequently, constant force is applied during double clamped bending simulation to caputre different behavior of hIAPP proto fibril. From double clamped bending simulation, we found that the difference in fracture toughness of polymorphic structures of hIAPP in spite of similar fracture process. Also we found the different number of hydrogen bonds which reveal the material's properties. Our simulation shows the different behavior of polymorphic structures due to different location of hydrophobic amino residues.

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