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# Nanomechanical behaviors and properties of amyloid fibrils

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**Abstract.** Amyloid fibrils have recently been considered as an interesting material, since they exhibit the excellent mechanical properties such as elastic modulus in the order of 10 GPa, which is larger than that of other protein materials. Despite recent findings of these excellent mechanical properties for amyloid fibrils, it has not been fully understood how these excellent mechanical properties are achieved. In this work, we have studied the nanomechanical deformation behaviors and properties of amyloid fibrils such as their elastic modulus as well as fracture strength, by using atomistic simulations, particularly steered molecular dynamics simulations. Our simulation results suggest the important role of the length of amyloid fibrils in their mechanical properties such that the fracture force of amyloid fibril is increased when the fibril length decreases. This length scale effect is attributed to the rupture mechanisms of hydrogen bonds that sustain the fibril structure. Moreover, we have investigated the effect of boundary condition on the nanomechanical deformation mechanisms of amyloid fibrils. It is found that the fracture force is critically affected by boundary condition. Our study highlights the crucial role of both fibril length and boundary condition in the nanomechanical properties of amyloid fibrils.

**Keywords:** amyloid fibrils; mechanical deformation mechanisms; molecular dynamics simulation; fracture property; boundary condition

## 1. Introduction

Amyloid fibrils, which are formed as a one-dimensional nanostructure via protein aggregation (Cherny and Gazit 2008), have been found to play a pivotal role in the pathogenesis of various diseases including neurodegenerative diseases (Pepys 2006, Hamley 2012) and type II diabetes (Hoppener *et al*. 2000). This indicates the necessity of understanding how the fibril structure is formed through self-assembly process, that is, protein aggregation (Straub and Thirumalai 2011). In the last decade, the molecular structure of amyloid fibril has been found to be stabilized through hydrogen bonding between protein chains, which are the aggregation-prone $\beta$-strand-rich structural motifs (Cherny and Gazit 2008). As it has recently been revealed that the $\beta$-strand-rich structural motif is able to effectively resist a mechanical force (Eom *et al*. 2003, Eom *et al*. 2005, Keten *et al*. 2010), it has been conjectured that amyloid fibril, which is composed of $\beta$-sheet-rich structural

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