Electronic Supplementary Material (ESI) for Soft Matter.

Coarse-Grained Molecular Model of Amyloid Fibrils Systems

Supplementary Information

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Amyloid fibril geometry and interactions

Our filament model (Figure S.1) consists of a twisting ribbon formed by two filaments of backbone beads that are bonded horizontally (r_0 = 1.000) and vertically (r_0=1.004). These values of r_0 arise naturally from the helicoidal geometry of the stranded fibril model. Similarly, bond bending parameters arise naturally from the geometry of the bi-stranded fibril model, which follows the equation of a helix. The intrinsic geometry of the model leads to the emergence of different θ_0 angles for backbone (bb) and interactive (ib) particles.

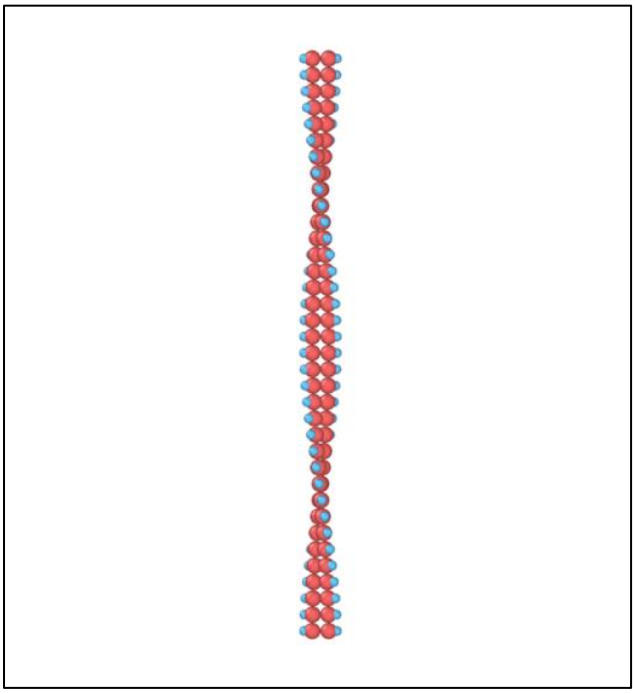

Figure S. 1: Coarse-grained d1 model representation of a two-filament twisting ribbon amyloid fibril.

The backbone (bb) and interactive (ib) particles serve different roles in our model. On one hand, the backbone (bb) particles model excluded volume interactions (short range repulsion) while the interactive (ib) particles represent the long-range electrostatic repulsion of amyloid fibrils in aqueous solution. For this reason, interactive (ib) particles are placed on the outer surface of backbone (bb) particles of the bi-stranded filament.

At this first stage of our model development, the short and long-range interactions are treated separately, thus a non-bonded interaction potential between interactive (ib) and backbone (bb) particles is not needed. However, bonded interactions between interactive (ib) and backbone (bb) particles are considered to maintain the geometry or bi-stranded structure of the filament.

Phase diagrams of the s1, s4, and d4 models

The phase diagrams of the other test models used in this work (s1, s4, d4) are presented in Figure S.2. The different liquid crystalline phases are colored from a qualitative perspective only to differentiate the different phases.

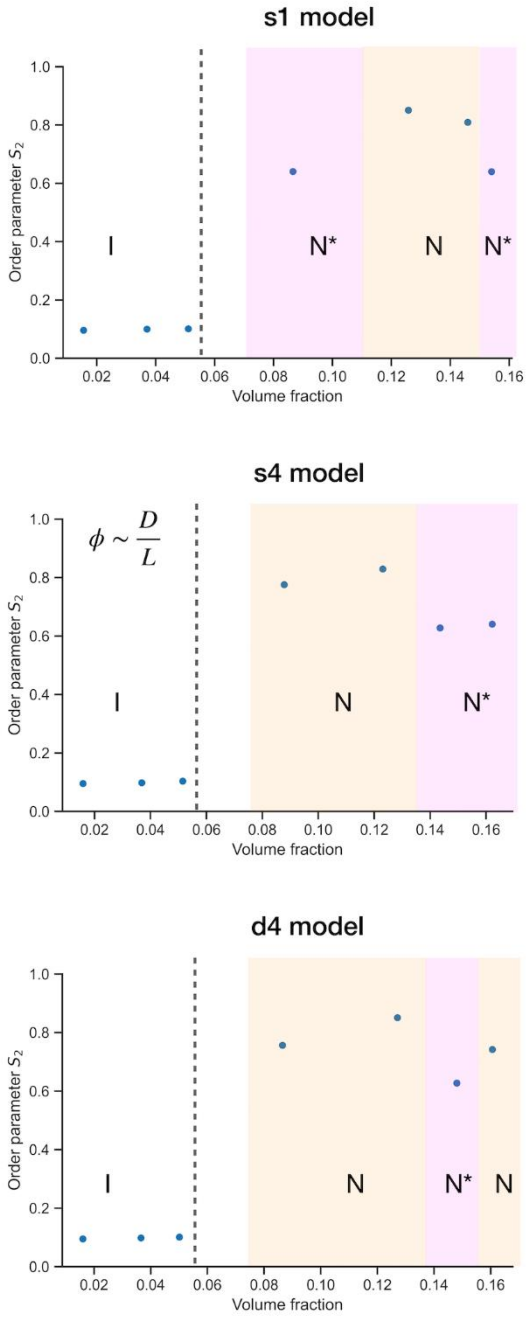

Figure S. 2: Phase diagrams of the s1, s4, and d4 models. Colors are used for qualitative differentiation of the different liquid crystalline phases.