Supporting information

Macroscale Assembly of Peptide Nanotubes

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(1) X-ray Powder Diffraction

![X-ray diffraction patterns of nanotubes before (a) and after (b) sulfate bundling.](image)

**Fig. S1.** Comparison of X-ray diffraction patterns of nanotubes before (a) and after (b) sulfate bundling. The typical cross-β conformation with ~5 Å and ~10 Å reflections are conserved. The presence of 9.4 Å reflection suggests the antiparallel β-sheet structure.

(2) Comparison of derived structure factors for nanotubes in salt solutions using form factors for a core-shell cylinder and a rectangular cross-section cylinder

The diameter of the nanotubes prior to bundling, 52 nm, and the repeat distance of 45.6 nm based on the first order peak at Q ~ 0.0138 Å−1 were used to determine the cross-section of the nanotubes. The tubes inside the bundles do not have a perfect square cross-section. Rather it fits better with a structure that is between a circle and a square, having square sides of length (l) and round edges of radius (r):

\[2r + l = 45.6\text{ (1)}\]

\[2r + 4l = 52\text{ nm}\]

Solving these simultaneous equations gives \(r = 11.09\text{ nm}\) and \(l = 23.42\text{ nm}\)
We compared the extracted structure factors using the form factors for core-shell cylinders with a circular ($r=26$ nm) and a square cross-section with $a = 41$ nm (Fig. 2S). In both cases, the peak positions are similar and consistent with a lamellar order.

**Core-shell circular cylinder form factor:**

![Diagram of a core-shell circular cylinder]

Eq. 1

$$F(q) = \frac{1}{\varphi} \int \int \left( (\rho_R - \rho_{\text{solute}}) R^2 \frac{qR\sin\alpha}{q\sin\alpha} + (\rho_s - \rho_R) r^2 \frac{2R(qr\sin\alpha)}{(qL\cos\alpha/2)} \right) \sin\alpha \cos\alpha \rho \vartheta d\alpha$$

**Generalized core-shell square cylinder form factor:**

![Diagram of a core-shell square cylinder]

Eq. 2

$$F(q) = \frac{2}{\psi} \int \int \left( (\rho_0 - \rho_{\text{solute}}) a_0 b_0 \phi(q, a_0, a_1, c_0, c_1, \alpha, \beta) + (\rho_1 - \rho_0) a_1 b_1 \phi(q, a_1, b_1, c_1, \alpha, \beta) \right) \sin\alpha \cos\alpha \psi \rho \vartheta$$

$$\psi = \left( (\rho_0 - \rho_{\text{solute}}) a_0 b_0 + (\rho_1 - \rho_0) a_1 b_1 \right)^2$$

$$\phi(q, a, b, c, \alpha, \beta) = \frac{\sin(qa\sin\alpha\cos\beta) \sin(qb\sin\alpha\sin\beta) \sin(qc\cos\alpha)}{qa\sin\alpha\cos\beta \ qb\sin\alpha\sin\beta \ qc\cos\alpha}$$
Fig. S2. Structure factor evaluations for different sulfate titrations using the form factors for core-shell cylinder with a circular cross-section (r=26 nm) and a square cross-section with a 41 nm width for the 9 mM sulfate titration. The peak intensity (red curve with markers for the 9 mM sulfate) is more pronounced, but the peak positions still correspond to the lamellar.