Supporting information

Macroscale Assembly of Peptide Nanotubes

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(1) X-ray Powder Diffraction

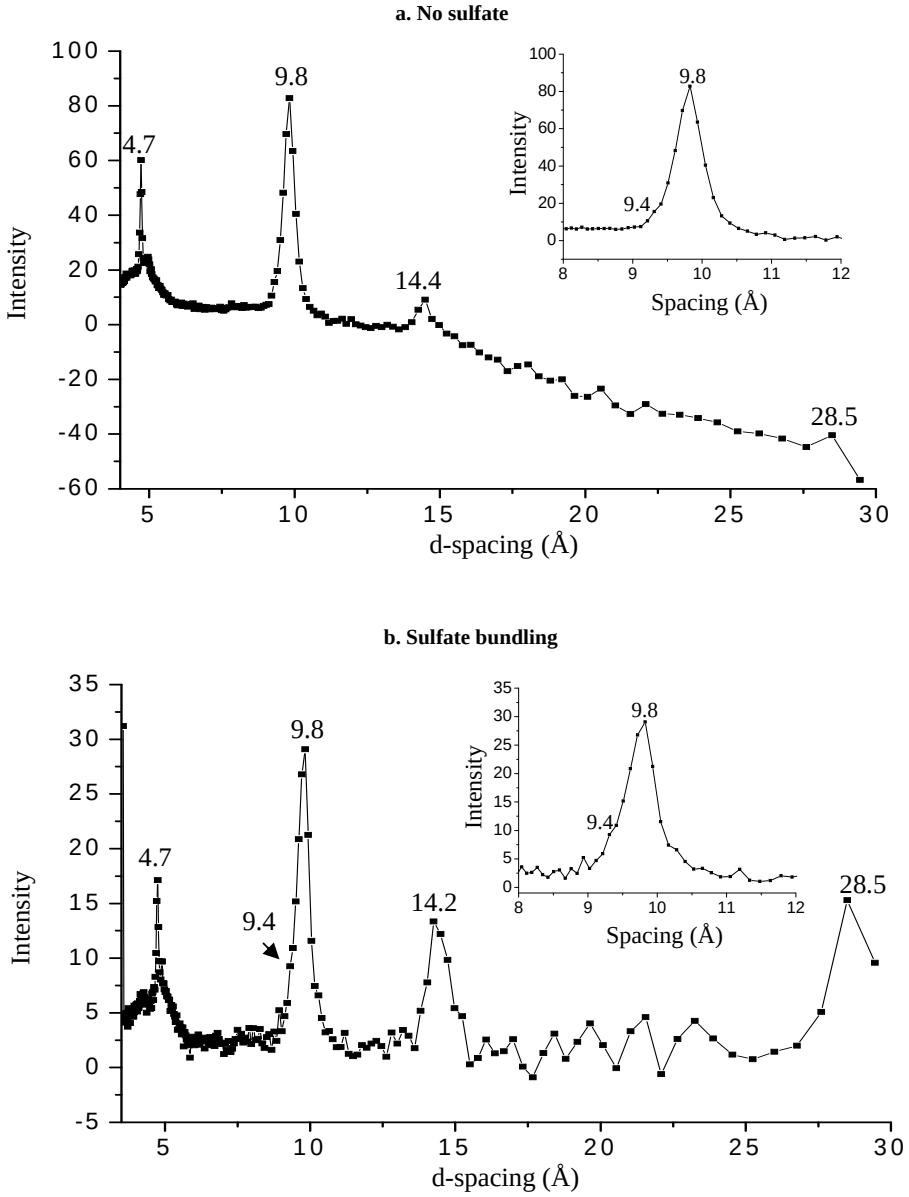


Fig. S1. Comparison of X-ray diffraction patterns of nanotubes before (a) and after (b) sulfate bundling. The typical cross-β conformation with ~ 5Å and ~ 10 Å reflections are conserved. The presence of 9.4 Å reflection suggests the antiparallel β-sheet structure.

(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} [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):

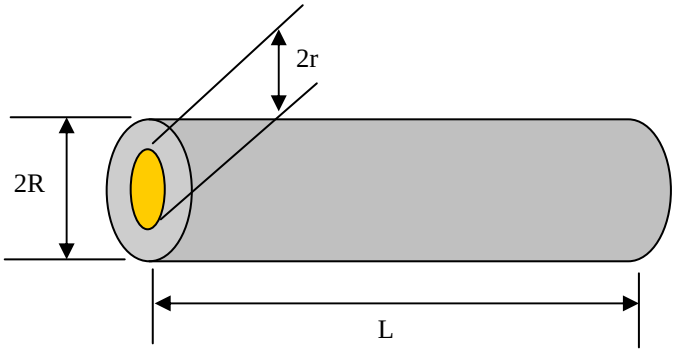
$$2r + l = 45.6 \quad (1)$$

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

Solving these simultaneous equations gives r = 11.09 nm and l=23.42 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:

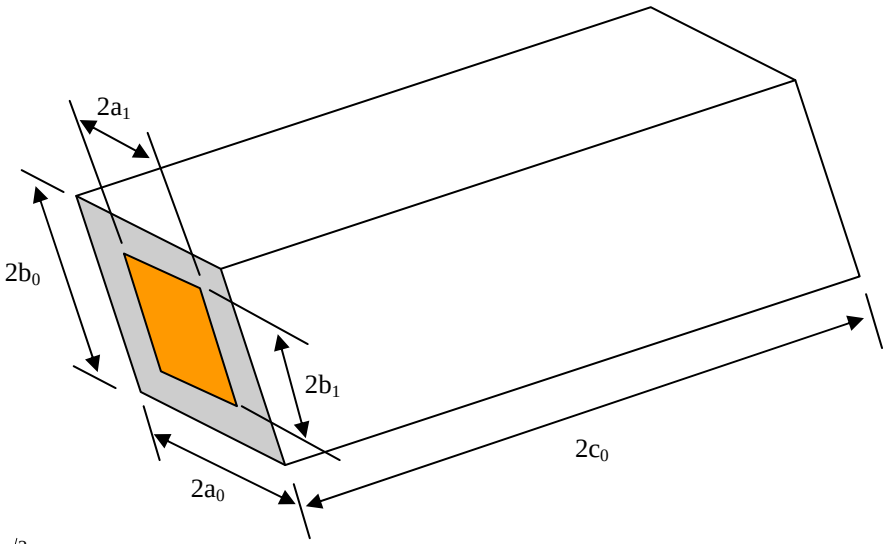


Eq. 1

$$F(q)=\frac{1}{\vartheta}\int_0^{\pi/2}\left[\left(\left(\rho_R-\rho_{solvent}\right)R^2\frac{2B_1\left(qR\sin\alpha\right)}{qR\sin\alpha}+\left(\rho_r-\rho_R\right)r^2\frac{2B_1\left(qr\sin\alpha\right)}{qr\sin\alpha}\right)\frac{\sin\left(\left(qL\cos\alpha\right)/2\right)}{\left(qL\cos\alpha\right)/2}\right]^2\sin\alpha d\alpha$$

$$\vartheta=\left[\left(\left(\rho_R-\rho_{solvent}\right)R^2+\left(\rho_r-\rho_R\right)r^2\right)\right]^2$$

Generalized core-shell square cylinder form factor:



Eq. 2

$$F(q)=\frac{2}{\pi\psi}\int_0^{\pi/2}\int_0^{\pi/2}\left(\left(\rho_0-\rho_{solvent}\right)a_0b_0\phi\left(q,a_0,b_0,c_0,\alpha,\beta\right)+\left(\rho_1-\rho_0\right)a_1b_1\phi\left(q,a_1,b_1,c_1,\alpha,\beta\right)\right)^2\sin\alpha d\alpha d\beta$$

$$\psi=\left(\left(\rho_0-\rho_{solvent}\right)a_0b_0+\left(\rho_1-\rho_0\right)a_1b_1\right)^2$$

$$\phi\left(q,a,b,c,\alpha,\beta\right)=\frac{\sin\left(qa\sin\alpha\cos\beta\right)}{qa\sin\alpha\cos\beta}\frac{\sin\left(qb\sin\alpha\sin\beta\right)}{qb\sin\alpha\sin\beta}\frac{\sin\left(qc\cos\alpha\right)}{qc\cos\alpha}$$

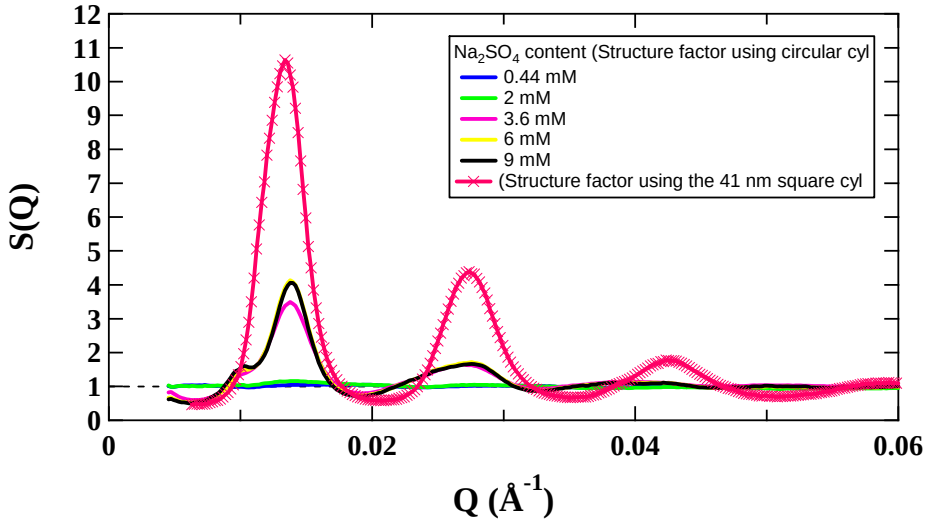


Fig. S2. Structure factor evaluations for different sulfate titrations using the form factors for core-shell cylinder with a circular cross-section (r=26 nm) and a square cross-section with a 41 nm width for the 9 mM sulfate titration. The peak intensity (red curve with markers for the 9 mM sulfate) is more pronounced, but the peak positions still correspond to the lamellar