Supporting Information for

Surface Effects on the Degree of Twist in Amyloid Fibril Structures

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Method

Materials. Amyloid-β peptide with 42 amphiphilic residues (DAEFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLMVGGVVIA) Aβ_{42} was purchased as lyophilized powder from Sigma-Aldrich. Its purity was confirmed by mass spectroscopy. 1-palmitoyl-2-oleoyl-glycero-3-phosphocholine (POPC) and cholesterol were purchased from Avanti Polar Lipids (Alabaster, AL, USA). All solvents used were reagent grade (Sigma-Aldrich). All chemicals were used as received without further purification. Phosphate-buffered saline (PBS) was freshly prepared from sodium and potassium salts: NaCl, KCl, Na_2HPO_4, and KH_2PO_4 to give a pH value of 7.4 at 25^{o}C.

Supported lipid bilayer (SLB). The SLB platforms were generated on freshly cleaned mica substrates. Briefly, each type of lipid/cholesterol mixtures with varying cholesterol molar-% (0, 2, 4, 5, 10, 20, 30, 40, 50 molar-%) was prepared in $CHCl_3$, dried, and re-suspended in PBS buffer (pH 7.4) to a concentration of 1.0 mg/mL. Suspension (~1 mL) of lipid/cholesterol mixture after pre-filtration was forced through a polycarbonate filter with 100 nm pores 11 times. Then, the mica substrates were immersed under the filtered lipid/cholesterol solutions (~500 μL) and incubated for one hour at room temperature under controlled humidity (~85%). Finally, the

excess vesicles in the solution phase were removed by extraction with fresh PBS buffer 10 times. The final volume of the solution was kept as ~500 μL.

Aβ_{42} peptide solutions. We prepared the peptide solution based on the previous reported method.[1,2] We first fully dissolved lyophilized Aβ_{42} in anhydrous dimethyl sulfoxide (DMSO) at a concentration of 1 mg/mL solution. The DMSO solution of Aβ_{42} was then diluted in a large amount of PBS (pH 7.4) to a final concentration of 1.0 μM. Finally, the solution was filtrated through a 20-nm membrane filter to remove the pre-existent aggregation of peptide molecules. The freshly prepared Aβ_{42} solution (1.0 μM) was used in all experiments. Note the 1.0 μM concentration used here is not only more than one order of magnitude lower than the critical micelle concentrations for Aβ_{42}, but also a factor of 2-15 lower than the reported post-aggregation solubility of Aβ_{42}. Thus, there is no pre-aggregation or fibril growth in the aqueous solution.

Aβ_{42} peptide fibrillation. For the fibril sample preparation, a home-made vial (1 mL) was chosen to incubate Aβ_{42} solutions. Before the fibril sample preparation, the SLB platforms were generated on freshly cleaned mica substrates inside the vial. About 500 μL of the freshly prepared Aβ_{42} solution (2.0 μM) was added into the vial containing ~500 μL PBS buffer and the SLB platform. The final concentration of Aβ_{42} was diluted to 1.0 μM. Then, the vial was sealed with a plastic cap to carefully eliminate the air bubble inside the vial. After incubation at 37 ^{o}C for 18 hrs, the mica substrate was carefully brought out, rinsed with pure water and allowed to dry in the air for further AFM characterization.

Atomic force microscope (AFM). The morphologies of amyloid fibrils on SLB formed on mica substrates were imaged on an atomic force microscopy (AFM, FM-Nanoview 1000) in a

tapping mode. A silicon tip on nitride level (Budget Sensors Inc.) with 48 N/m spring constant and 190 kHz resonance frequency was used. To more accurately analyze the twisting fibrils, we used an opensource fibril-fitting software called FiberApp[3] on multiple AFM images to add representative line sections running parallel to the long axis of the fibril. Up to 500 crossover sections on every surface are analyzed to give each histogram.

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[1] Shezad, K.; Zhang, K.; Hussain, M.; Dong, H.; He, C.; Gong, X.; Xie, X.; Zhu, J.; Shen, L. Surface Roughness Modulates Diffusion and Fibrillation of Amyloid-β Peptides. *Langmuir* **2016**, *32*, 8238-8244.

[2] Shen, L.; Adachi, T.; Vanden Bout, D.; Zhu, X. Y. A Mobile Precursor Determines Amyloid-β Peptide Fibril Formation at Interfaces. *J. Am. Chem. Soc.* **2012**, *134*, 14172-14178.

[3] Usov, I; Mezzenga, R. FiberApp: An Open-Source Software for Tracking and Analyzing Polymers, Filaments, Biomacromolecules, and Fibrous Objects. *Macromolecules* **2015**, *48*, 1269-1280.