

Supplementary Information

Unravelling the non-classical nucleation mechanism of an amyloid nanosheet through atomic force microscopy and an infrared probe technique

Yao Wang^{‡,a}, Ziqi Wang^{‡,a}, Lujuan Yang^a, Wenkai Zhang^{*,b}, and Gang Ma^{*,a}

^aKey Laboratory of Medicinal Chemistry and Molecular Diagnosis of Ministry of Education, Key Laboratory of Analytical Science and Technology of Hebei Province, State Key Laboratory of New Pharmaceutical Preparations and Excipients, Hebei Research Center of the Basic Discipline of Synthetic Chemistry, College of Chemistry and Materials Science, Hebei University, Baoding 071002, China. E-mail: gangma@hbu.edu.cn

^bDepartment of Physics, Applied Optics Beijing Area Major Laboratory, Center for Advanced Quantum Studies, Beijing Normal University, Beijing 100875, China. E-mail: wkzhang@bnu.edu.cn

*corresponding author

‡equal contribution

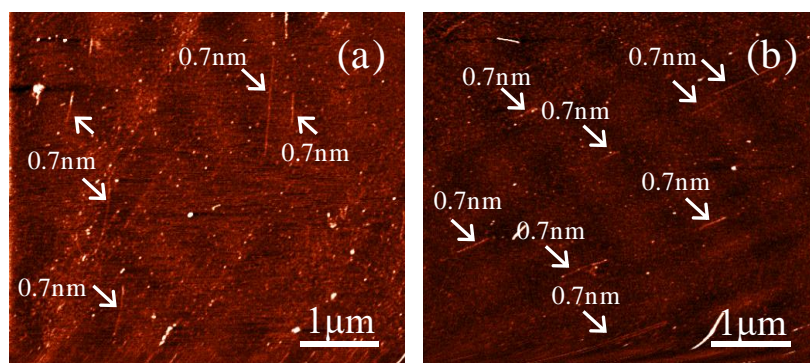


Fig. S1. AFM morphology characterizations of the KLVFXAK system during amyloid nanosheet formation as a function of incubation time: (a) $t=3$ min; (b) $t=6$ min.

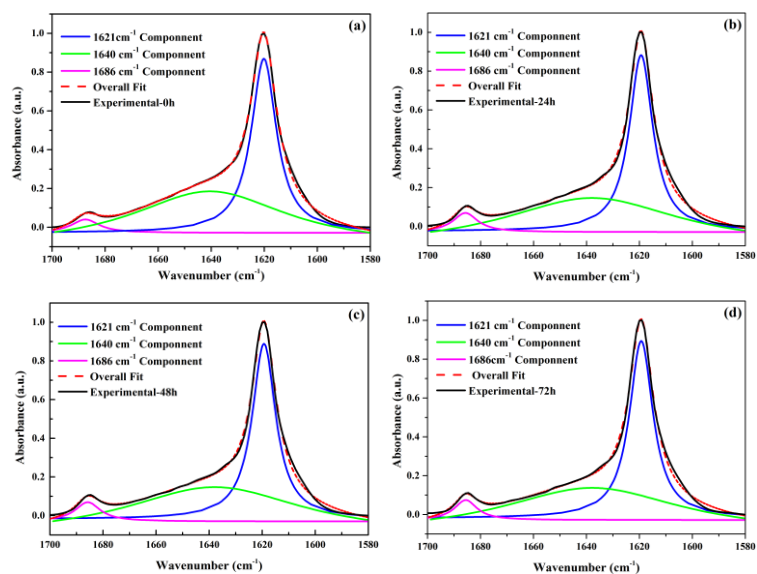


Fig. S2. Curve-fitting results of the FTIR spectra at different time points of the KLVFXAK system during the nanosheet formation in the amide I region. (a) $t=0$ h; (b) $t=24$ h; (c) $t=48$ h; (d) $t=72$ h.

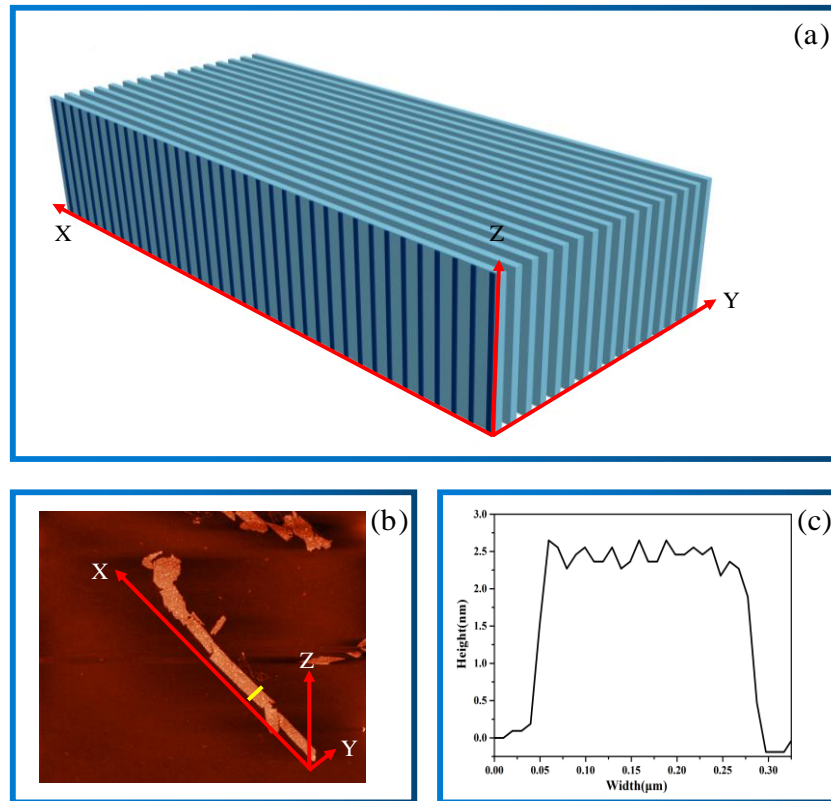


Fig. S3. Comparative illustration of the proposed model and experimental AFM image for KLVFXAK nanosheet under the same coordinate system. (a) Model; (b) AFM ; (c) AFM height curve of the yellow cross section in (b).

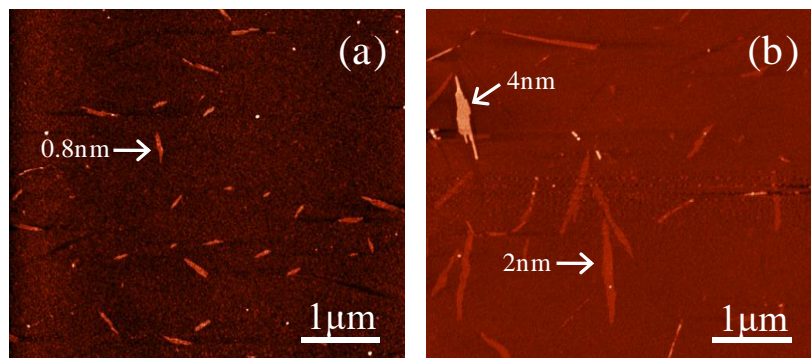


Fig. S4. AFM morphology characterizations of the KLVFXAE system during amyloid nanosheet formation as a function of incubation time: (a) $t=5$ min; (b) $t=15$ min.

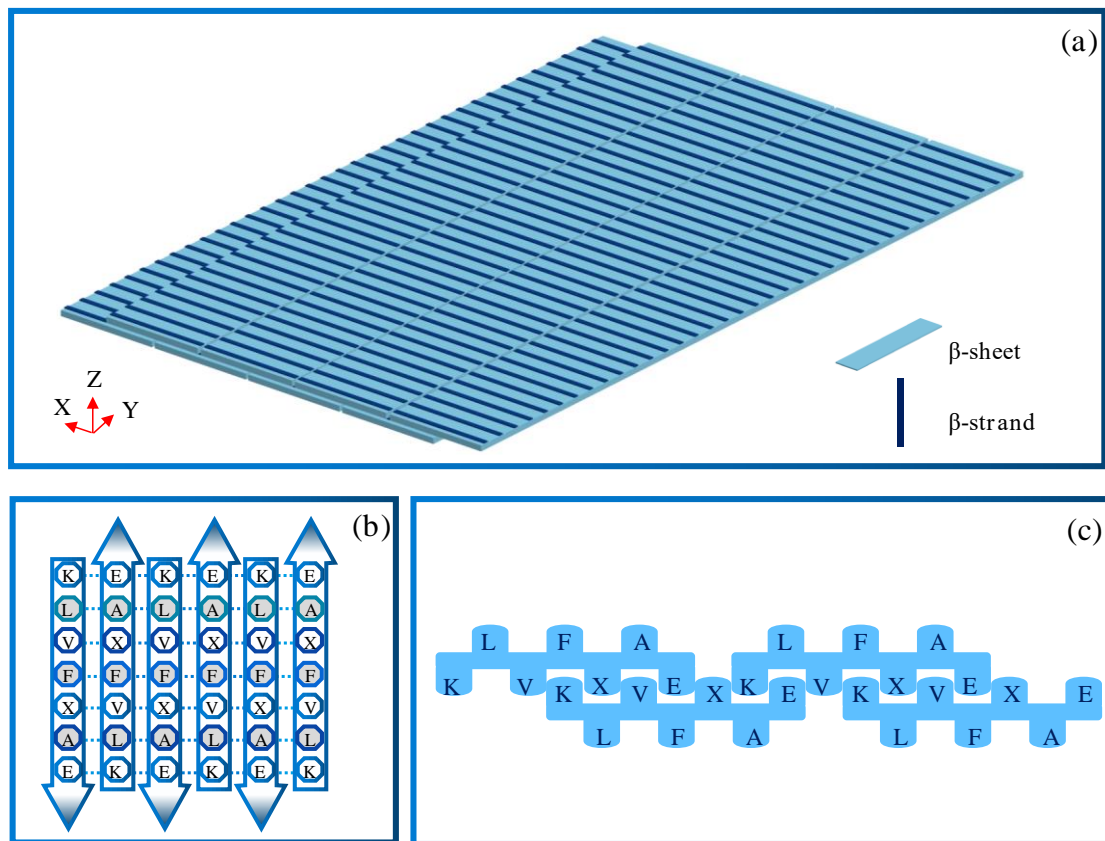


Fig. S5. Structural model of KLVFXAE nanosheet: (a) Overview of the model. Each dark-blue stripe represents an individual KLVFXAE β -strand and each light-blue sheet represents an individual KLVFXAE antiparallel β -sheet; (b) View towards the X-Y plane where the viewer can see the details of the KLVFXAE antiparallel β -sheet; each arrow represents an individual KLVFXAE β -strand (from N terminal to C terminal) and six strands are shown as representatives; octagon with letter: amino acid residue; open octagon: residue with its side chain pointing towards the viewer; shaded octagon: residue with its side chain pointing away from the viewer; (c) View towards the X-Z plane where the viewer can see how X₂₀ is H-bonded by neighboring K₁₆ and the presence of the electrostatic interaction between oppositely charged peptide terminals (i.e. between NH₃⁺ and COO⁻).

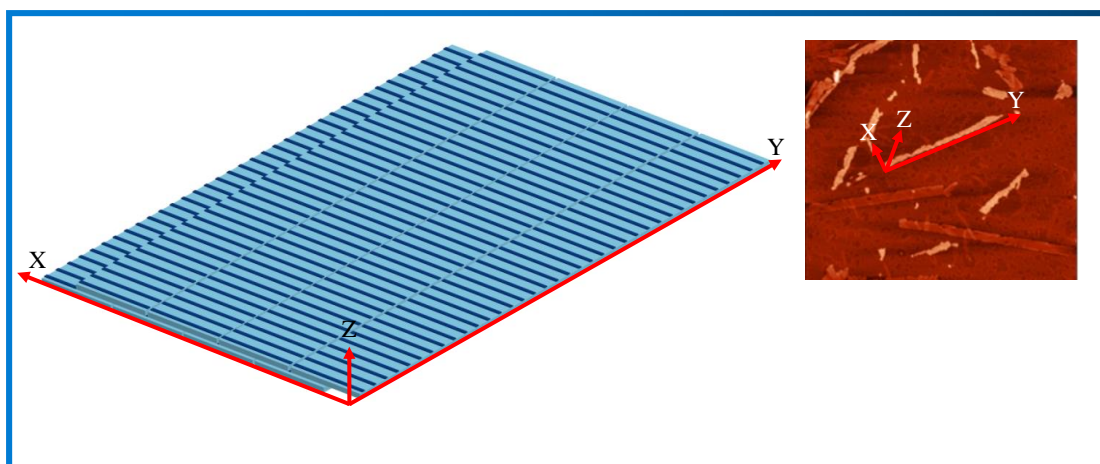


Fig. S6. Comparative illustration of the proposed model and experimental AFM image for KLVFXAE nanosheet under the same coordinate system. (a) Model; (b) AFM.