Electronic Supplementary Material (ESI) for Soft Matter.

Formation of protein-mediated bilayer tubes is governed by a snapthrough transition

Electronic Supplementary Information

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A Model Development

A.1 Surface representation

In a polar coordinate the membrane can be parameterized by the arclength s and the rotation angle θ as

$$\boldsymbol{r}(r, z, \theta) = \boldsymbol{r}(s, \theta). \tag{S1}$$

The surface tangents are given by $\boldsymbol{e}_s = \boldsymbol{r}_{,s}$ and $\boldsymbol{r}_{,\theta}$. The surface metric $a_{ij} = \boldsymbol{e}_i \cdot \boldsymbol{e}_j$ becomes

$$a_{ij} = \begin{bmatrix} 1 & 0 \\ 0 & r^2 \end{bmatrix}. \tag{S2}$$

The curvature tensor $b_{ij} = e_{i,j} \cdot \boldsymbol{n}$ simplifies to

$$b_{ij} = \begin{bmatrix} \psi_s & 0 \\ 0 & r \sin\psi \end{bmatrix}. \tag{S3}$$

The mean curvatures is given by

$$H = \frac{1}{2} a^{\alpha\beta} b_{\alpha\beta},$$

where, $a^{\alpha\beta}$ is the inverse of the metric tension. The principal curvature can be extracted from the curvature tensor as

$$c_\zeta = b_{\alpha\beta} \zeta^\alpha \zeta^\beta,$$

and

$$c_\mu = b_{\alpha\beta} \mu^\alpha \mu^\beta.$$

where, $\boldsymbol{\zeta}$ and $\boldsymbol{\mu}$ are surface tangents in two principal directions, The deviatoric curvature becomes

$$D = \frac{1}{2}(c_\zeta - c_\mu).$$

A.2 Protein Orientation

The orientation of a protein [1] on the surface can be represented by orientation unit vector $\boldsymbol{\zeta}$ (Figure S1) which essentially indicates tangent to the curve on which protein orients [2]. Thus we can constitute another unit vector $\boldsymbol{\mu}$, such that: $\boldsymbol{\mu} = \boldsymbol{n} \times \boldsymbol{\zeta}$.

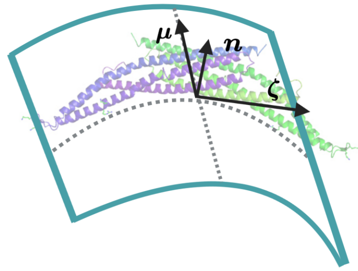

Figure S1: Orientation vectors of BAR-domain proteins

A.3 Balance relations

The force balance equation is dictated by

$$\boldsymbol{T}^{\alpha}_{;\alpha} + p\boldsymbol{n} = \boldsymbol{0}\,, \tag{S4}$$

where p is normal pressure on the membrane and $\boldsymbol{T}$ is traction on the membrane and given by,

$$\boldsymbol{T}^{\alpha} = N^{\beta\alpha}\boldsymbol{a}_{\beta} + S^{\alpha}\boldsymbol{n}. \tag{S5}$$

Here, $\boldsymbol{N}$ is the in-plane component of the stress and is given by

$$N^{\beta\alpha} = \zeta^{\beta\alpha} + b^{\beta}_{\mu}M^{\mu\alpha} \qquad \text{and} \qquad S^{\alpha} = -M^{\alpha\beta}_{;\beta}\,, \tag{S6}$$

where $\sigma^{\beta\alpha}$ and $M^{\beta\alpha}$ are obtained from the following constitutive relations [3]

$$\sigma^{\beta\alpha} = \rho\left(\frac{\partial F}{\partial a_{\alpha\beta}} + \frac{\partial F}{\partial a_{\beta\alpha}}\right) \quad \text{and} \quad \boldsymbol{M}^{\beta\alpha} = \frac{\rho}{2}\left(\frac{\partial F}{\partial b_{\alpha\beta}} + \frac{\partial F}{\partial b_{\beta\alpha}}\right), \tag{S7}$$

with $F = W/\rho$ as the energy mass density of the membrane. Combining these we get the balance equations in tangent and normal direction

$$N^{\beta\alpha}_{;\alpha} - S^{\alpha}b^{\beta}_{\alpha} = 0, \quad S^{\alpha}_{;\alpha} + N^{\beta\alpha}b_{\beta\alpha} + p = 0 \tag{S8}$$

The normal force balance relation in Equation S8_{ii} becomes [2]

$$\begin{aligned} &\underbrace{\frac{1}{2}[W_{,D}(\zeta^{\alpha}\zeta^{\beta} - \mu^{\alpha}\mu^{\beta})]_{;\beta\alpha}}_{\text{I}} + \underbrace{\frac{1}{2}W_{,D}(\zeta^{\alpha}\zeta^{\beta} - \mu^{\alpha}\mu^{\beta})b_{\alpha\gamma}b^{\gamma}_{\beta}}_{\text{II}} + \\ &\Delta\left(\frac{1}{2}W_{,H}\right) + (W_{,K})_{;\beta\alpha}\left(2Ha^{\beta\alpha} - b^{\beta\alpha}\right) + W_{,H}(2H^2 - K) + 2H(KW_{,K} - W) - 2H\lambda = p, \end{aligned} \tag{S9}$$

where the marked terms are simplified in the next section for an axisymmetric geometry. To construct a force boundary condition we use the expression of the normal traction force as given by [4]

$$\begin{aligned} F_n = &(\tau W_K)' - \frac{1}{2}(W_H)_{,\nu} - (W_K)_{,\beta}\,\tilde{b}^{\alpha\beta}v_{\alpha} \\ &+ \frac{1}{2}(W_D)_{,\nu} - \left(W_D\lambda^{\alpha}\lambda^{\beta}\right)_{;\beta}v_{\alpha} - \left(W_D\lambda^{\alpha}\lambda^{\beta}v_{\beta}\tau_{\alpha}\right)', \end{aligned} \tag{S10}$$

where $\boldsymbol{\tau}$ is the unit tangent to the curve at boundary, $\boldsymbol{\nu}$ is the outward normal to the same curve at the boundary, and can be constructed from local surface normal $\boldsymbol{n}$ as $\boldsymbol{\nu} = \boldsymbol{\tau} \times \boldsymbol{n}$.

B Simplification in axisymmetry

B.1 Governing equations

We have orthogonal surface tangent vectors as given by

$$\boldsymbol{a}_1 = \boldsymbol{e}_s, \quad \boldsymbol{a}_2 = r\boldsymbol{e}_{\theta}. \tag{S11}$$

We get the expression of orientation unit vector in terms of orthogonal basis vectors as given below

$$\boldsymbol{\zeta} = -\boldsymbol{e}_\theta = -\frac{1}{r}\boldsymbol{a}_2, \quad \boldsymbol{\mu} = \boldsymbol{a}_1. \tag{S12}$$

We first find the expressions of the direct products of orientation vectors used in Equation (S9) below

$$\zeta^\alpha \zeta^\beta = \begin{pmatrix} 0 & 0 \\ 0 & 1/r^2 \end{pmatrix}, \tag{S13}$$

and

$$\mu^\alpha \mu^\beta = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}. \tag{S14}$$

In the limit of axisymmetry, the components of Christoffel symbols denoted by

$$\Gamma^a_{bc} = \frac{1}{2} a^{ad} \left[\partial_a a_{bd} + \partial_b a_{dc} - \partial_d a_{bc} \right].$$

The components of the Christoffel are given below with 1 and 2 denoting the arclength (s) and azimuthal direction, respectively

$$\begin{array}{l} \Gamma^1_{11} = 0, \quad \Gamma^2_{22} = 0, \quad \Gamma^1_{22} = -r\cos\psi, \\ \Gamma^2_{12} = \Gamma^2_{21} = \frac{\cos\psi}{r}, \quad \Gamma^1_{21} = 0, \text{and} \quad \Gamma^2_{11} = 0. \end{array} \tag{S15}$$

We first simplify the term I in Equation (S9) below

$$\begin{aligned} \mathrm{I} &= \frac{1}{2}\left[W_D \left(\zeta^\alpha \zeta^\beta - \mu^\alpha \mu^\beta \right) \right]_{;\beta\alpha} \\ &= (W_{,D}\zeta^\alpha\zeta^\beta)_{;\beta\alpha} - \frac{1}{2}\left[W_D \left(\zeta^\alpha \zeta^\beta + \mu^\alpha \mu^\beta \right) \right]_{;\beta\alpha} \\ &= (W_{,D}\zeta^\alpha\zeta^\beta)_{;\beta\alpha} - \frac{1}{2}(W_{,D} a^{\alpha\beta})_{;\beta\alpha}. \end{aligned} \tag{S16}$$

Note that we recover the surface metric from the addition of the direct products of the orientation vectors as given below

$$\left(\zeta^\alpha \zeta^\beta + \mu^\alpha \mu^\beta \right) = \begin{pmatrix} 1 & 0 \\ 0 & 1/r^2 \end{pmatrix} = a^{\alpha\beta}. \tag{S17}$$

From Equation S16 we can further write term I as

$$\begin{aligned} \mathrm{I} &= (W_{,D}\zeta^\alpha\zeta^\beta)_{;\beta\alpha} - \frac{1}{2}\Delta(W_{,D}) \\ &= \eta^\beta_{;\beta} - \frac{1}{2}\Delta(W_{,D}), \end{aligned} \tag{S18}$$

where

$$\begin{aligned} \eta^\beta &= \left(W_D \zeta^\alpha \zeta^\beta \right)_{;\alpha} \\ &= \left(W_{,D} \zeta^\alpha \zeta^\beta \right)_{,\alpha} + W_{,D}\Gamma^\alpha_{\alpha\gamma}\zeta^\gamma\zeta^\beta + W_{,D}\Gamma^\beta_{\alpha\gamma}\zeta^\alpha\zeta^\gamma. \end{aligned} \tag{S19}$$

The components of η^β are estimated below in two principal directions

$$\eta^1 = 0 + 0 + W_{,D}\Gamma^1_{22}\zeta^2\zeta^2 = -\frac{\cos\psi}{r}W_{,D}, \tag{S20}$$

and

$$\eta^2 = 0 + 0 + 0 = 0. \tag{S21}$$

The divergent $\eta^\beta_{;\beta}$ reduces to

$$\begin{aligned} \eta^\beta_{;\beta} &= \frac{1}{\sqrt{a}}(\sqrt{a}\eta^\beta)_{,\beta} \\ &= \frac{1}{r}(r\eta^1)_{,1} \\ &= -\frac{(\cos\psi W_{,D})'}{r}. \end{aligned} \tag{S22}$$

Substituting the expression of $\eta^{\beta}_{;\beta}$ in Equation S16 we get term I simplified as

$$\mathrm{I} = -\frac{1}{2}\Delta(W_{,D}) - \frac{(\cos\psi W_{,D})'}{r}. \tag{S23}$$

Next, we simplify term II below

$$\begin{aligned}\mathrm{II} &= \frac{1}{2}W_D\left(\zeta^{\alpha}\zeta^{\beta} - \mu^{\alpha}\mu^{\beta}\right)b_{\alpha\gamma}b^{\gamma}_{\beta}\\ &= \frac{1}{2}W_D\left\{\zeta^2\zeta^2 b_{22}b^2_2 - \mu^1\mu^1 b_{11}b^1_1\right\}\\ &= \frac{1}{2}W_{,D}\left\{\frac{\sin^2\psi}{r^2} - \psi'^2\right\}\\ &= \frac{1}{2}W_{,D}\left(\frac{\sin\psi}{r} + \psi'\right)\left(\frac{\sin\psi}{r} - \psi'\right)\\ &= \frac{1}{2}W_{,D}\;2H\;2D\\ &= 2HDW_{,D}.\end{aligned} \tag{S24}$$

Finally, using the simplifications of term I (Equation (S23)) and term II (Equation (S24)), the shape equation becomes

$$p = \frac{L'}{r} + W_H\left(2H^2 - K\right) - 2H\left(W + \lambda - W_D D\right), \tag{S25}$$

where L relates to the expression of the traction as shown in Equation (S10), given by

$$L/r = \frac{1}{2}\left[(W_H)' - (W_D)'\right] - \frac{\cos\psi}{r}W_{,D} = -F_n. \tag{S26}$$

The above relation gives a natural boundary condition for L at the center and the boundary. At the center it directly correlates with the value of pulling force as

$$p_f = \lim_{r\longrightarrow 0} 2\pi r F_n = -2\pi L(0). \tag{S27}$$

Note than the derivation of shape equation was presented in [2] where the last term was missing in the definition of L/r in Equation (S26) and which led to an incorrect residual term $\frac{(W_D)'\cos\psi}{r}$ in the shape equation. Please note that an artificial pulling force was introduced for the boundary condition of $L = 0$ at the center of the membrane with the incomplete expression as presented in Walani et al. [2].

B.2 Area parameterization

The governing equation is solved on a patch of membrane with fixed surface area, where the coat area of protein is prescribed. The arclength parametrization poses some difficulty since total arclength varies depending on the equilibrium shape of the membrane. Therefore, we did a coordinate transformation of arclength to a local area a as given by

$$\frac{\partial}{\partial s} = 2\pi r\frac{\partial}{\partial a}. \tag{S28}$$

Note that in the differential form local area relates as

$$da = 2\pi r ds \tag{S29}$$

The tangential force balance relation in Equation 7 transforms to

$$\frac{\partial\lambda}{\partial a} = 2\kappa(H - C_0)\frac{\partial C_0}{\partial a} + 2\kappa_d(D - D_0)\frac{\partial D_0}{\partial a}. \tag{S30}$$

The normal force balance relation in Equation 8 becomes

$$p = 2\pi\frac{\partial L}{\partial a} + 2\kappa(H - C_0)\left(2H^2 - K\right) - 2H\left(W + \lambda - 2\kappa_d D(D - D_0)\right) \tag{S31}$$

where,

$$\frac{L}{r} = \pi r\frac{\partial}{\partial a}\Big\{\kappa(H - C_0) - \kappa_d(D - D_0)\Big\} - 2\kappa_D(D - D_0)\frac{\cos\psi}{r}. \tag{S32}$$

B.3 Non-dimensionalization

In this section we use $\tilde{(\cdot)}$ to represent the dimensionless quantities. We used a scale of curvature $1/R_0$, where R_0 is the equivalent lengthscale in the domain. The dimensionless mean, deviatoric and Gaussian curvature becomes $\tilde{H} = R_0 H$, $\tilde{D} = R_0 D$, and $\tilde{K} = R_0^2 K$. The same scale for curvature is used to nondimensionalize spontaneous mean and deviatoric curvatures and they become $\tilde{C}_0 = R_0 C_0$ and $\tilde{D}_0 = R_0 D_0$. The area is dimensionalized with scale $A_0 = 2\pi R_0^2$. The scale for membrane tension is taken as κ/R_0^2, therefore $\tilde{\lambda} = R_0^2 \lambda/\kappa$. The dimensionless form of L becomes $\tilde{L} = R_0 L/\kappa$.
The tangential force balance relation in Equation (S30) reads as

$$\frac{\partial \tilde{\lambda}}{\partial \tilde{a}} = 2(\tilde{H} - \tilde{C}_0)\frac{\partial \tilde{C}_0}{\partial \tilde{a}} + 2\tilde{\kappa}_d(\tilde{D} - \tilde{D}_0)\frac{\partial \tilde{D}_0}{\partial \tilde{a}}, \tag{S33}$$

where $\tilde{\kappa}_d = \frac{\kappa_d}{\kappa}$ represents the dimensionless deviatoric curvature. The normal force balance relation in Equation (S31) simplifies to

$$\tilde{p} = \frac{\partial \tilde{L}}{\partial \tilde{a}} + 2(\tilde{H} - \tilde{C}_0)\left(2\tilde{H}^2 - \tilde{K}\right) - 2\tilde{H}\Big\{(\tilde{H} - \tilde{C}_0)^2 + \tilde{\kappa}_d(\tilde{D} - \tilde{D}_0)^2 + \tilde{\lambda} - 2\tilde{\kappa}_d\tilde{D}(\tilde{D} - \tilde{D}_0)\Big\}, \tag{S34}$$

with

$$\frac{\tilde{L}}{\tilde{r}} = \tilde{r}^2 \frac{\partial}{\partial \tilde{a}}\Big\{(H - C_0) - \tilde{\kappa}_d(D - D_0)\Big\} - 2\tilde{\kappa}_d(D - D_0)\frac{\cos\psi}{r}. \tag{S35}$$

C Supplementary Figures

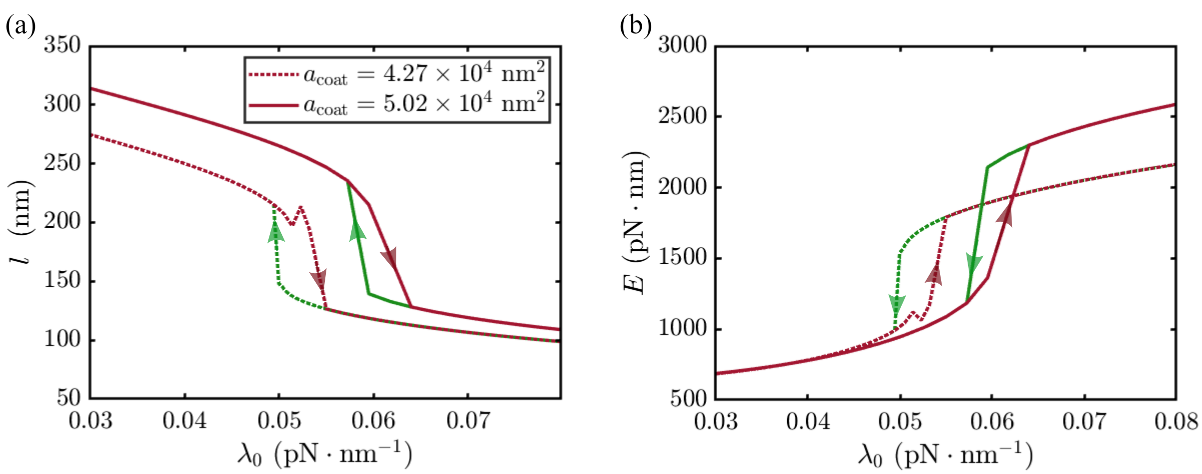

Figure S2: Forward and backward transition to demonstrate snapthrough instability. (a) Transition of tube length in the direction of increasing and decreasing membrane tension for $D_0 = 0.017\ \text{nm}^{-1}$ and $\kappa = 168\ \text{pN}\cdot\text{nm}$ and two different values of coat area of proteins. (b) Transition of bending energy in the direction of increasing and decreasing membrane tension for $D_0 = 0.017\ \text{nm}^{-1}$ and $\kappa = 168\ \text{pN}\cdot\text{nm}$ and two different values of coat area of proteins.

References

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