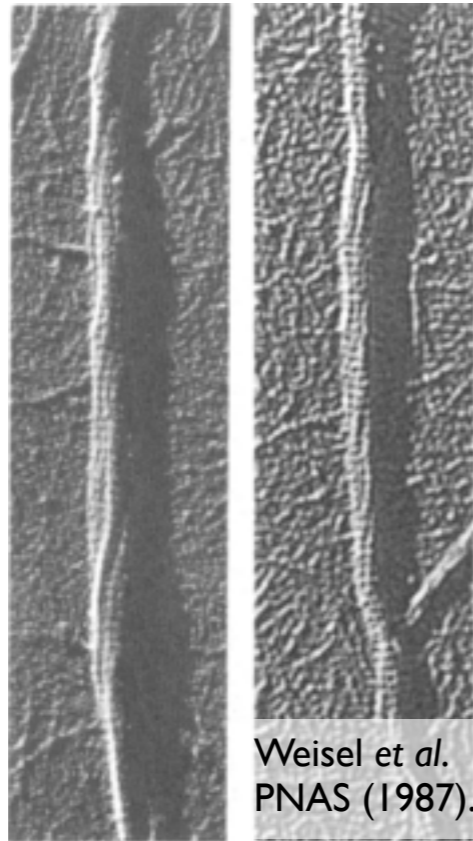


# Surveying the metric geometry of filamentous matter: Defects and instabilities of incompatible bundles

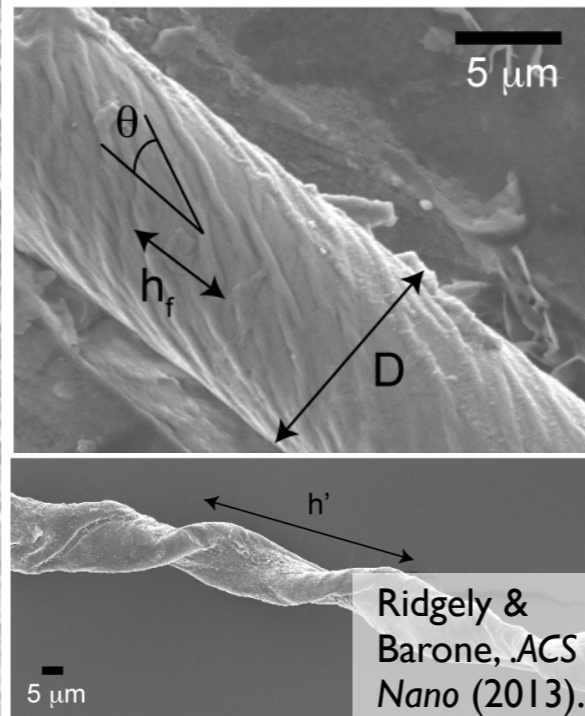
**collagen fibrils**



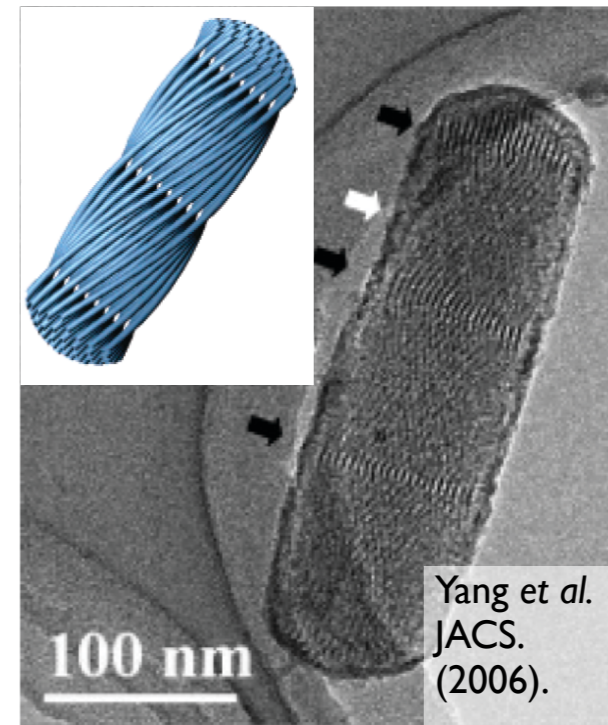
**fibrin bundles**



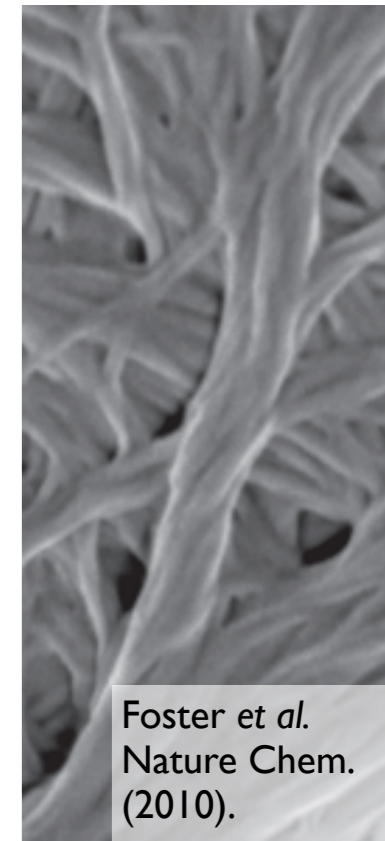
**amyloid fibrils**



**mesoporous silica  
(columnar micelles)**



**organogel fibers**



Isaac Bruss, Amir Azadi, Doug Hall & **Gregory M. Grason**

Department of Polymer Science & Engineering  
University of Massachusetts Amherst

<http://www.pse.umass.edu/ggrason>



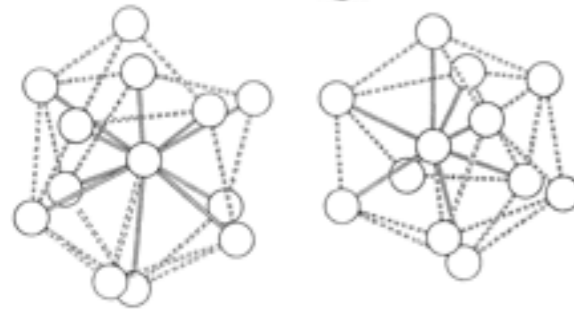
NSF CAREER DMR 09-55760; Alfred P. Sloan Foundation;  
UMass Center for Hierarchical Manufacturing (NSF NSEC)





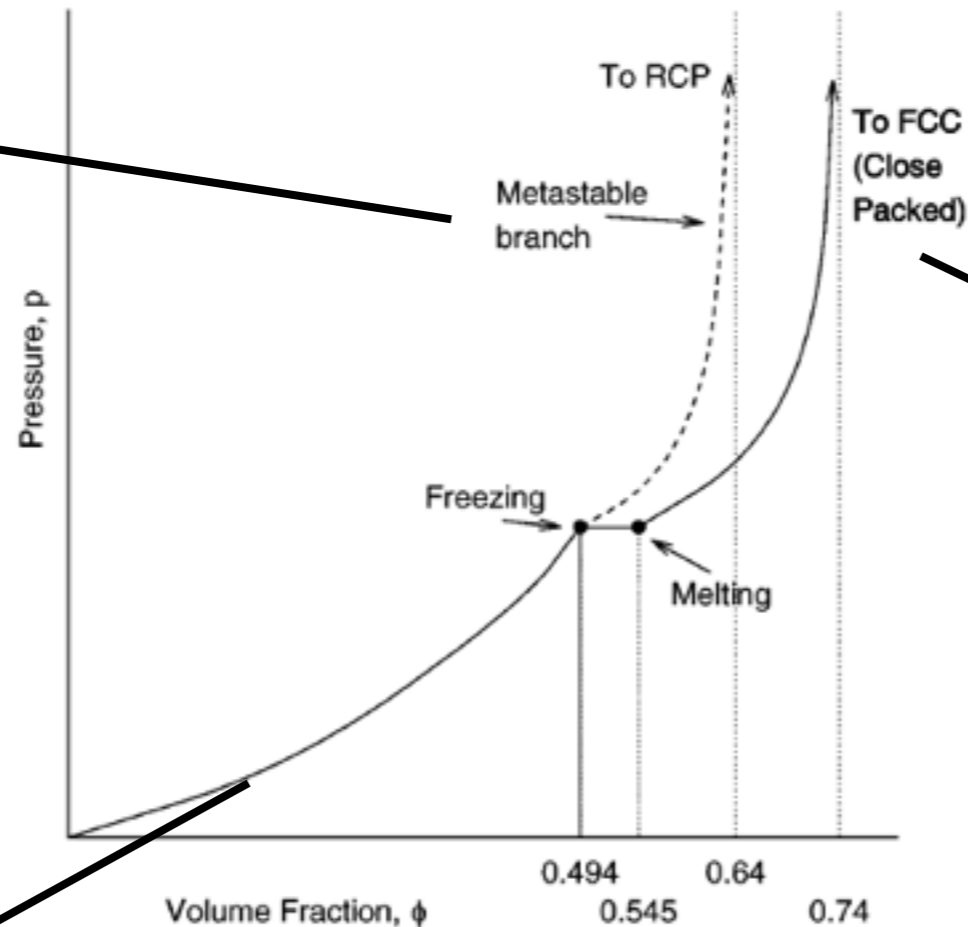
# Models of matter: Spheres from Kepler to colloids

random-close packing:  
from dense liquids to glassiness



Bernal, *Nature* (1960).

equation of state hard spheres

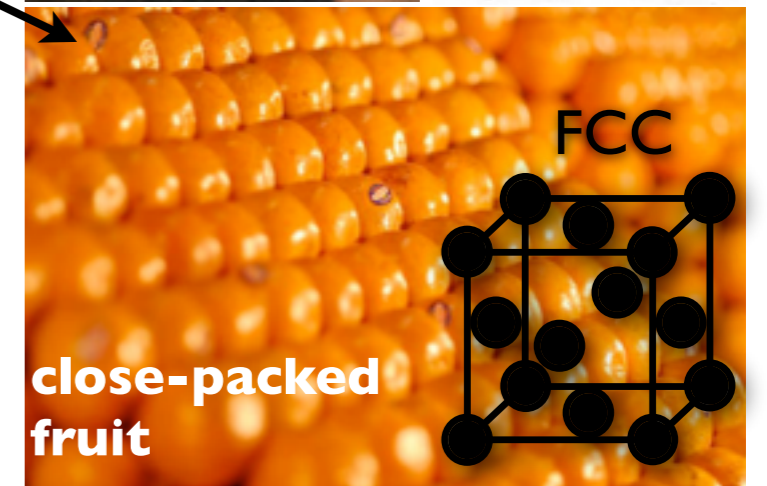
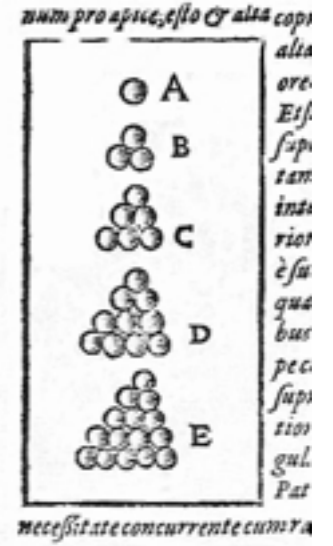


Rintoul & Torquato, *PRL* (1996).

sphere packing, optimal lattices  
& crystallization



Kepler (1611)

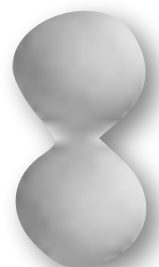


close-packed fruit

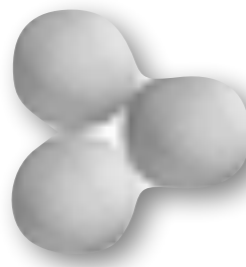


silica particles  
(colloidal x-tal)

**N-body cluster geometry  
& viral expansion**



2-sphere



3-sphere



4-sphere



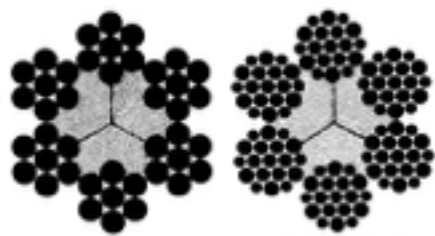
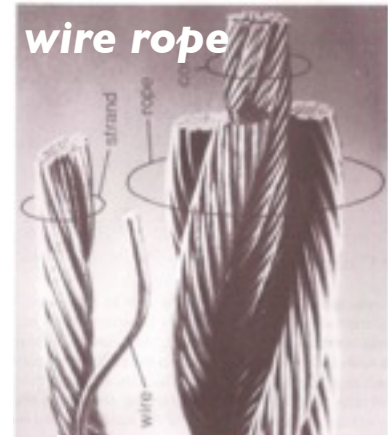
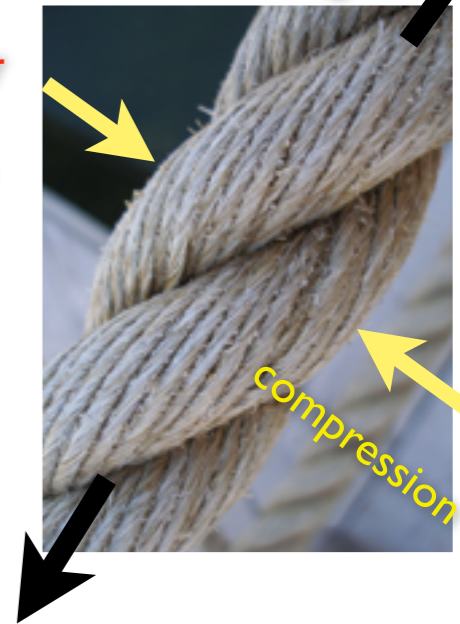
# Models of matter: Filamentous matter from Galileo to nanomaterials

macroscale,  
manufactured  
materials

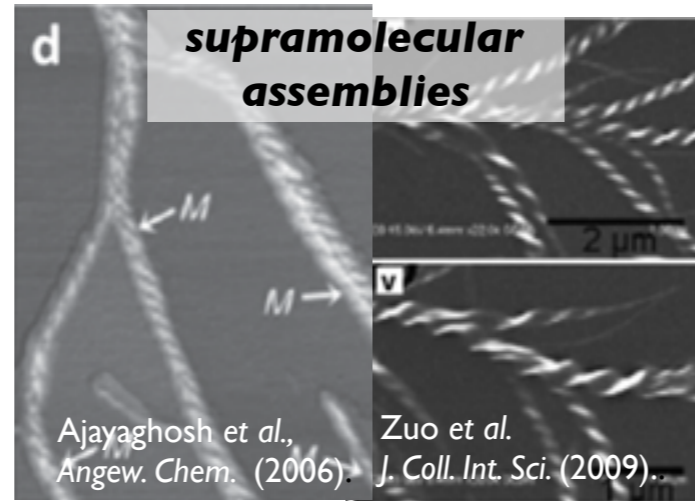


“But in the case of the rope, the **very act of twisting causes the threads to bind one another** in such a way that when the rope is stretched with a great force, the fibers break rather than separate from each other.”

Galileo, *Strength of Materials* (1638)



(~0.1-1m diameter)



supramolecular  
assemblies

Ajayaghosh et al.,  
*Angew. Chem.* (2006).

Zuo et al.  
*J. Coll. Int. Sci.* (2009).

nanoscale self-assembled  
materials

(~10-1000 nm “rope” diameter;  
~1-10 nm “filament” diameter)

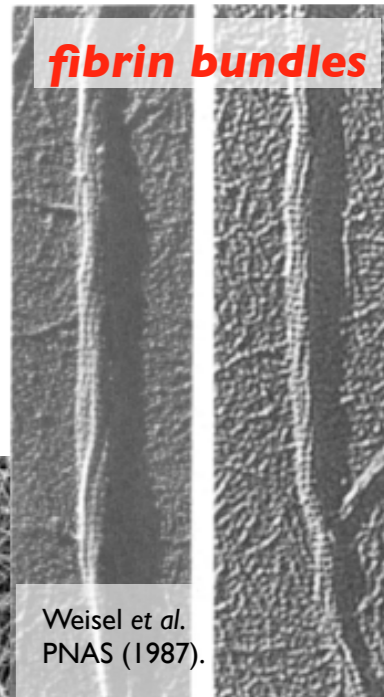


(~0.1-1cm  
diameter)

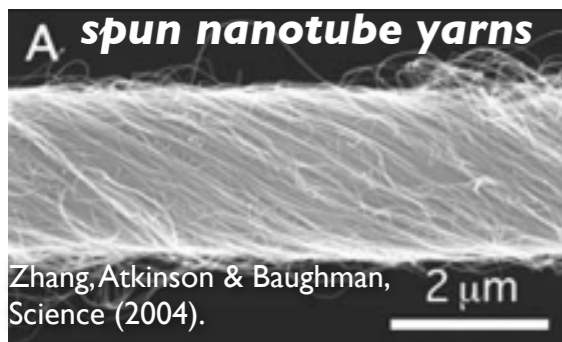
yarns &  
textiles



fibrin bundles



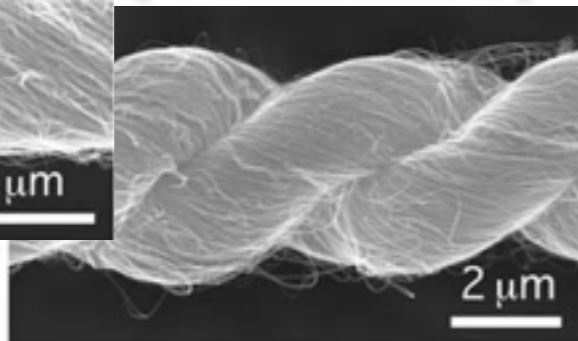
Weisel et al.  
*PNAS* (1987).



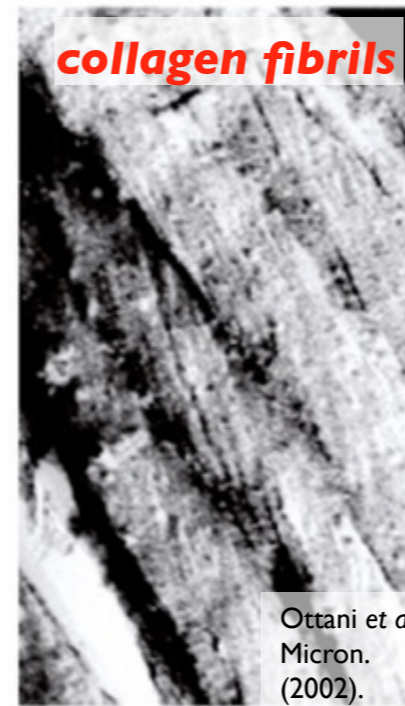
Zhang, Atkinson & Baughman,  
*Science* (2004).

2 μm

(~1 micron diameter)

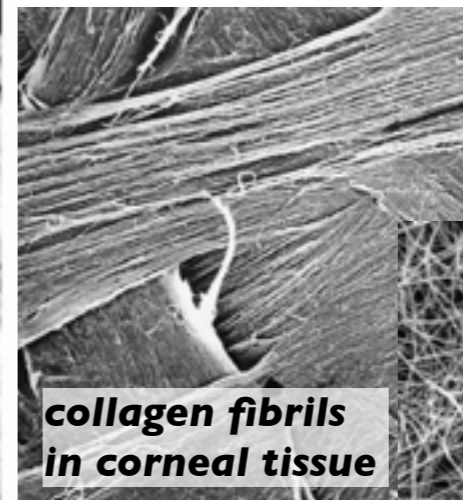


2 μm

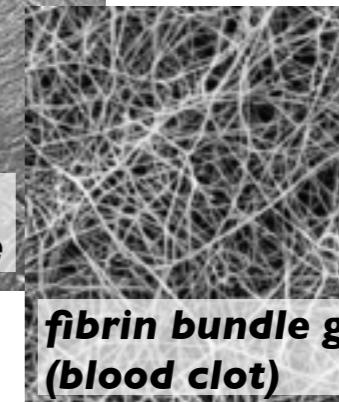


collagen fibrils

Ottani et al.  
*Micron.*  
(2002).



collagen fibrils  
in corneal tissue



fibrin bundle gel  
(blood clot)



# Generic challenges to understanding cohesive filament assembly

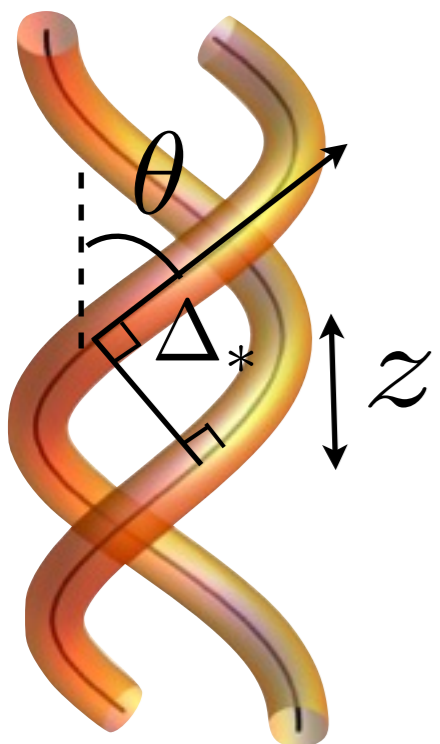
- 1) Extreme aspect ratio ( $L/d \gg 1$ )  
→ extreme *flexibility* relative to *inter-filament cohesion*

$$E_{mech} \approx \frac{B}{2} L \kappa^2 \quad (B \sim d^4)$$

bending stiffness

$$E_{coh} \approx -\epsilon L$$

- 2) “Distance” and contact are *non-local* → coupling between *orientation* & *spacing*



Distance of  
closest approach:

$$\Delta_* = \min_z [\Delta(z)]$$



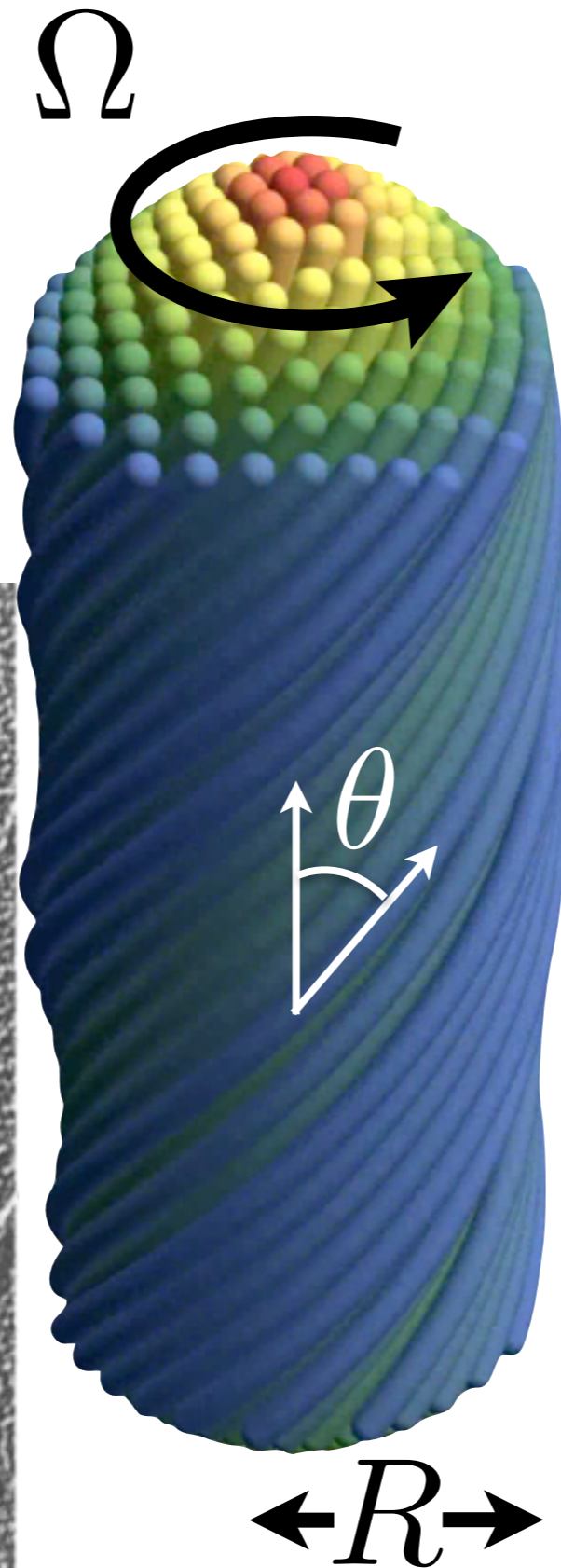
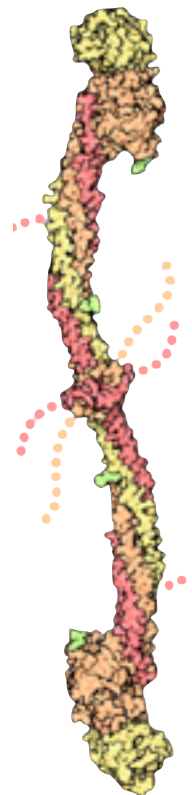
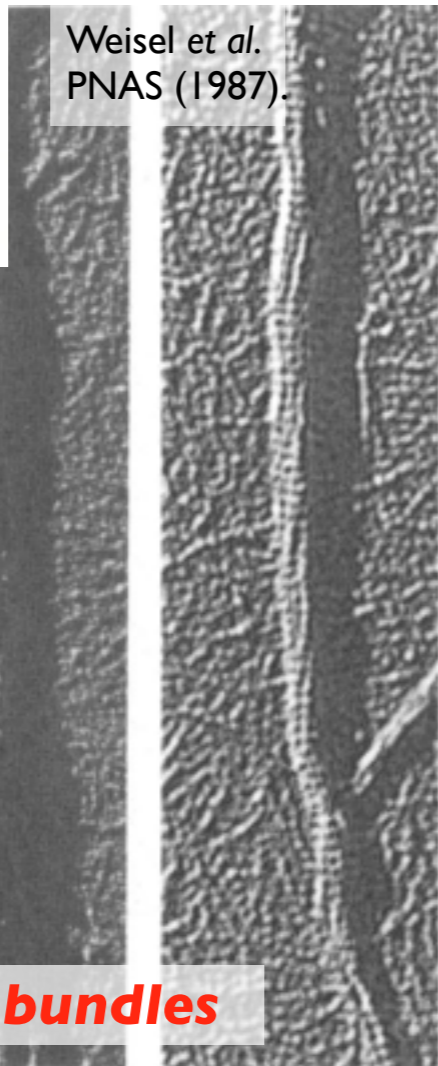
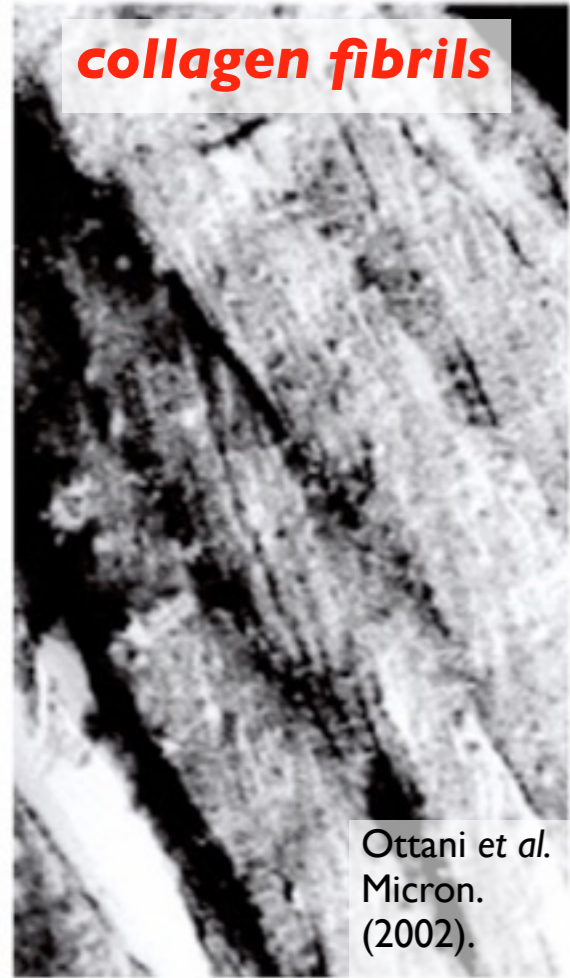
## Broad Questions:

How does 3D shape (e.g. **twist**, **bend**) of a multi-filament assembly (e.g. bundle) influence structure & energetics of lateral order?

What are optimal packings for non-trivial bundle geometry? What determines these?



# Structure & assembly of twisted, cohesive bundles



## Motivations:

- 1) “Self-twisting” *chiral filament bundle*: common structural motif of biofilament assemblies
- 2) Twist: Simplest, non-trivial example of coupling between filament tilt and spacing

$R$  - radius

$\Omega$  - helical rotation rate ( $2\pi/\text{pitch}$ )

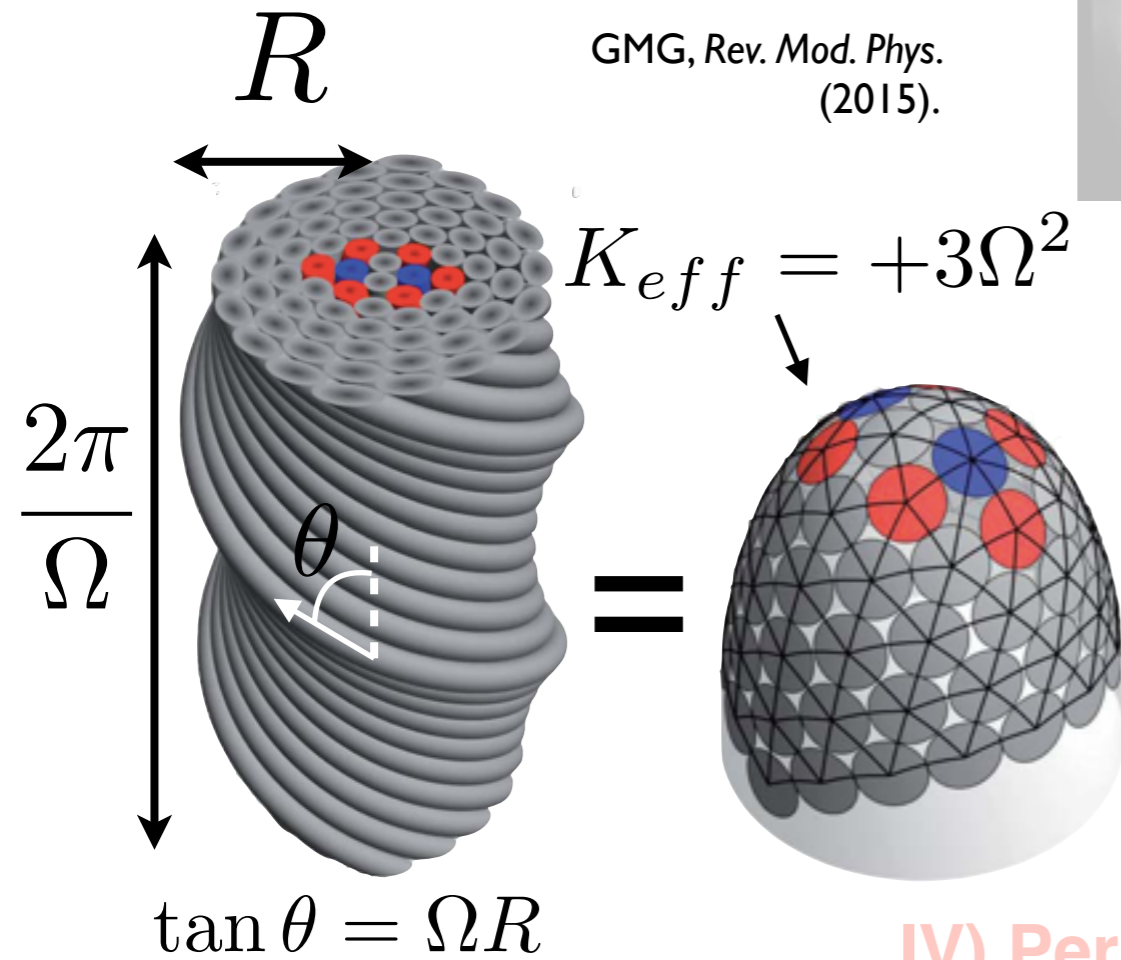
$$\tan \theta = \Omega R$$

$\theta$  - helical tilt angle

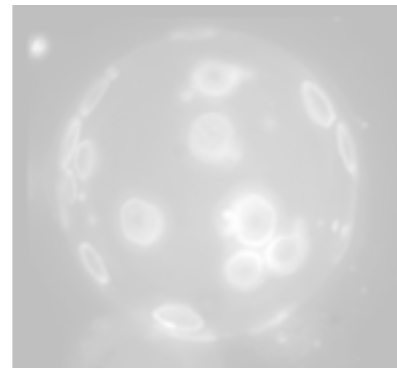


# Twisted bundles: non-Euclidean geometry & anomalous assembly

## I) Non-euclidean "metric" geometry of bundles

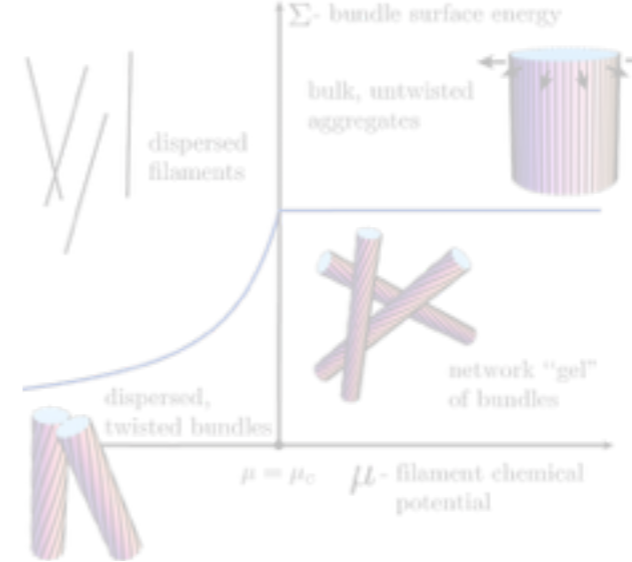


solid domains on lipid vesicles



Bandekar & Sofou, *Langmuir* (2012)

chiral filament assembly

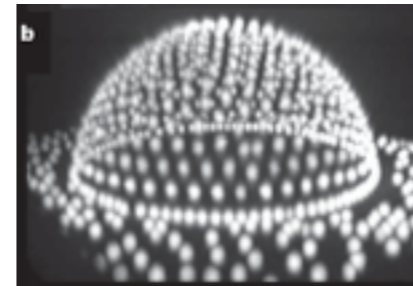


## II) Self-limiting Assembly

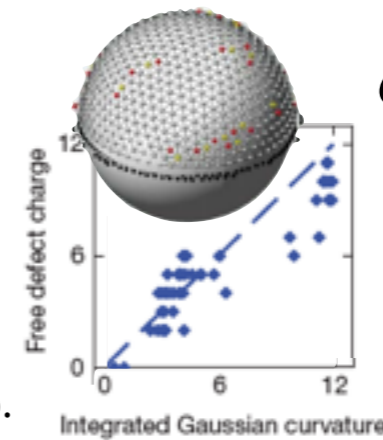
GMG & Bruinsma, *PRL* (2007); GMG, *PRE* (2009)

## III) Topological Defects

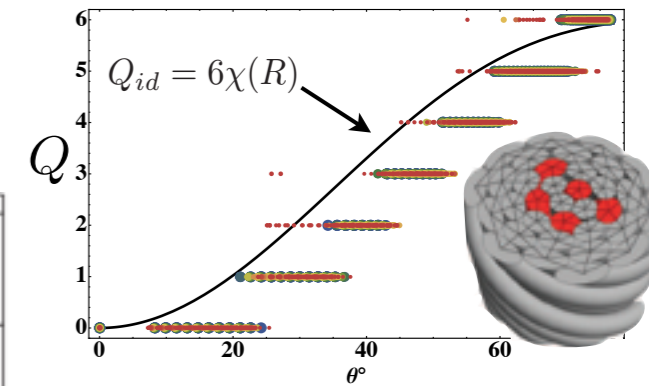
defects in curved crystals



Irvine et al., *Nature* (2010).



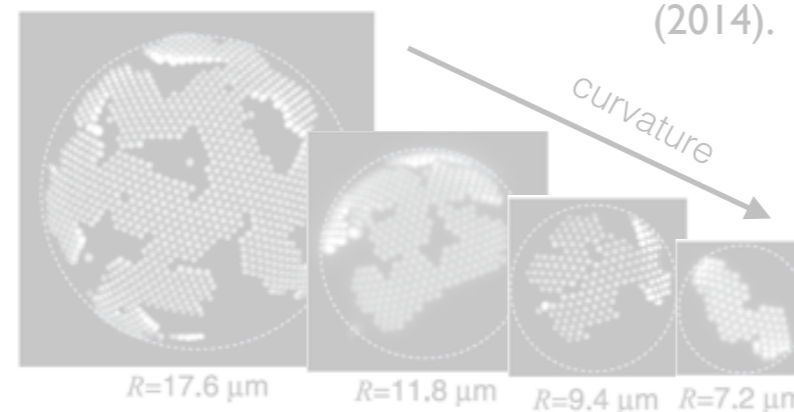
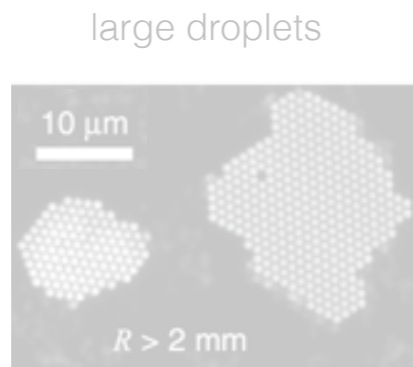
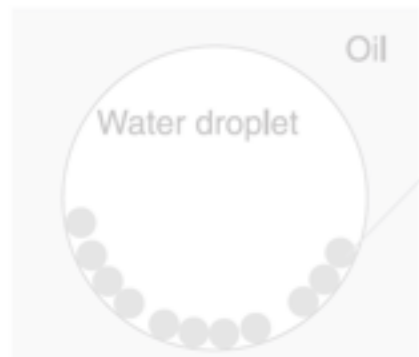
defects in twisted bundles



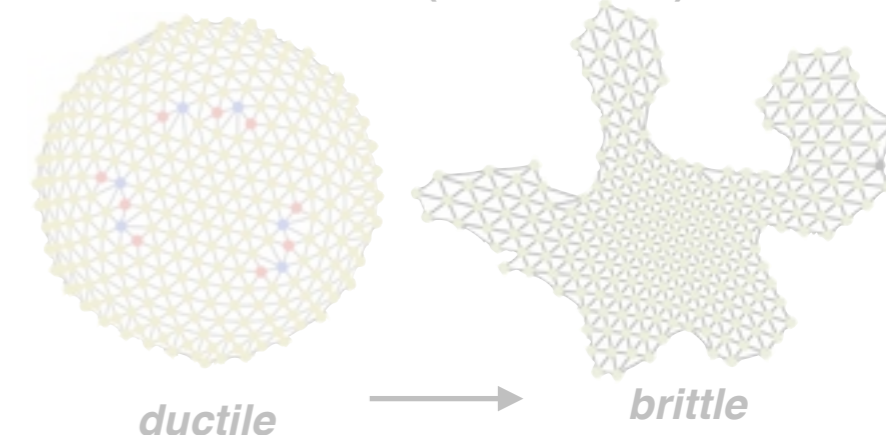
Bruss & GMG, *PNAS* (2012); *Soft Matter* (2013).

## IV) Perimeter Instability & Anisotropic Domains

colloidal crystals on spherical droplets



cohesive membranes on spherical substrates (simulations)

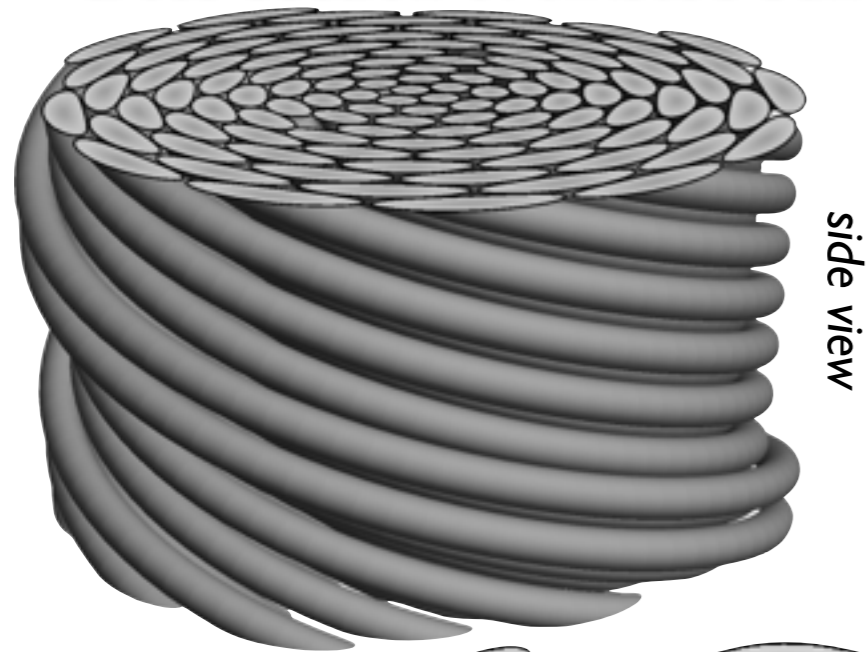


Amir Azadi, to be published.

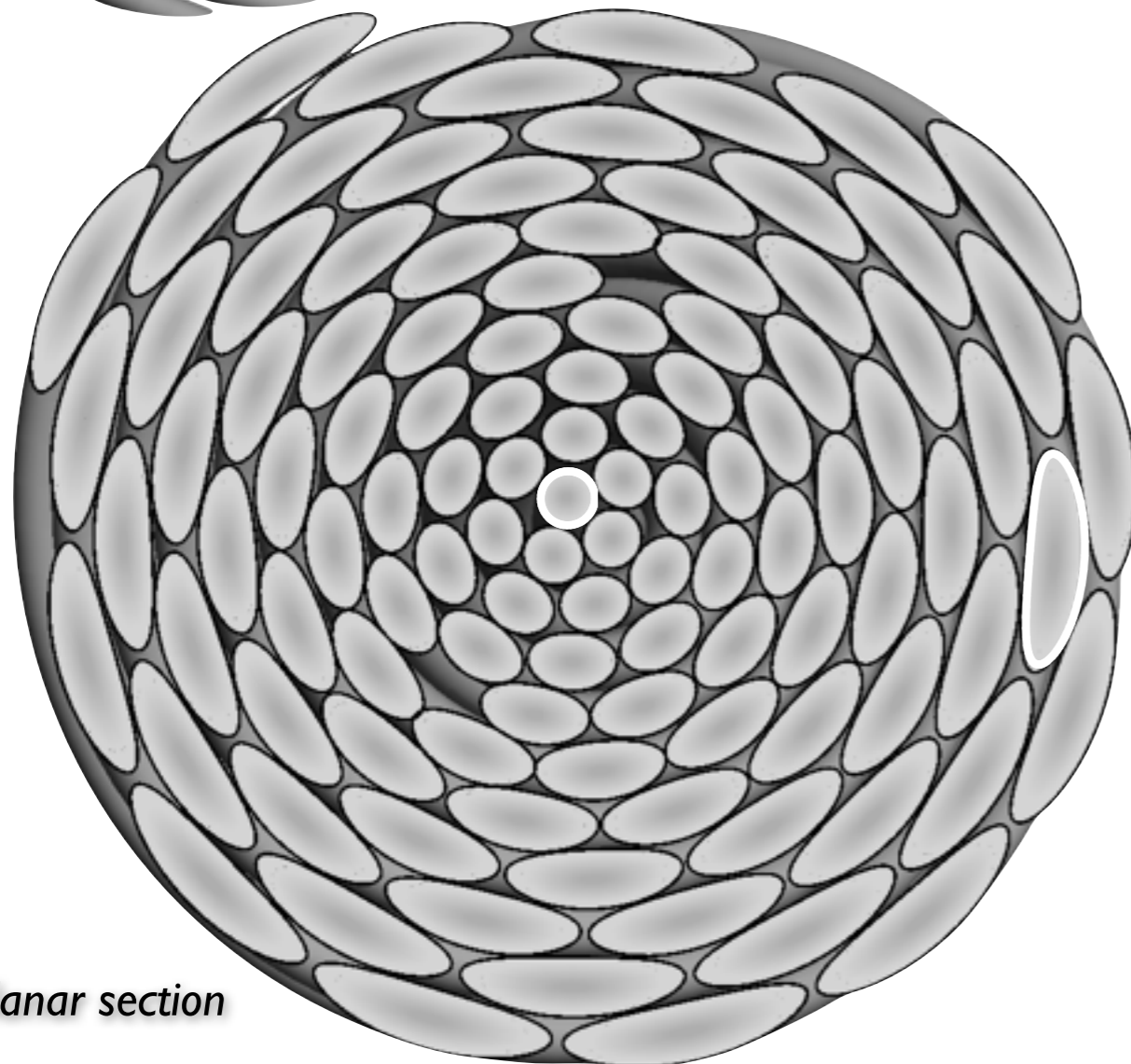


# Mapping frustration in filament packing

cross-section of twisted bundle

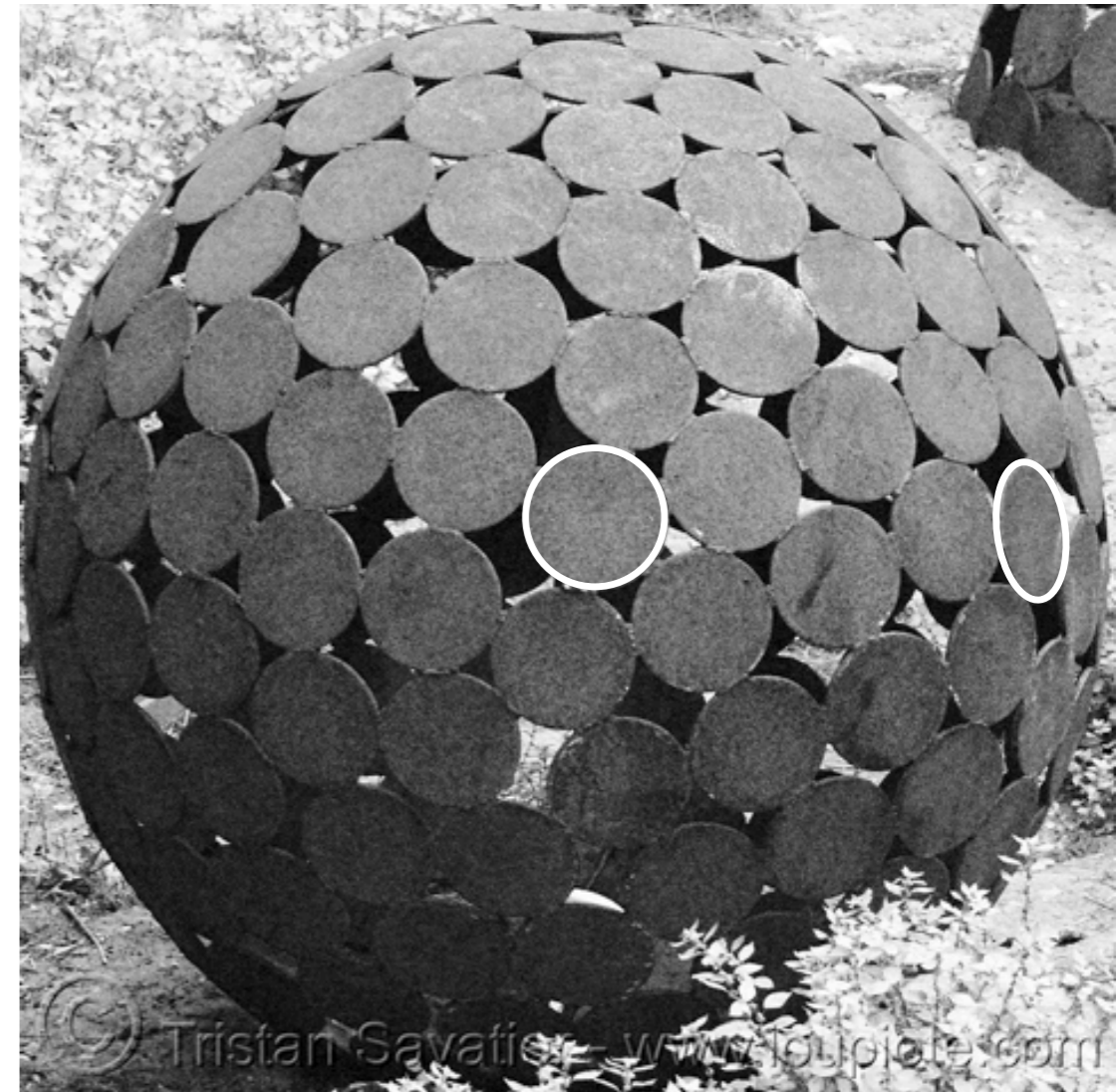


side view



planar section

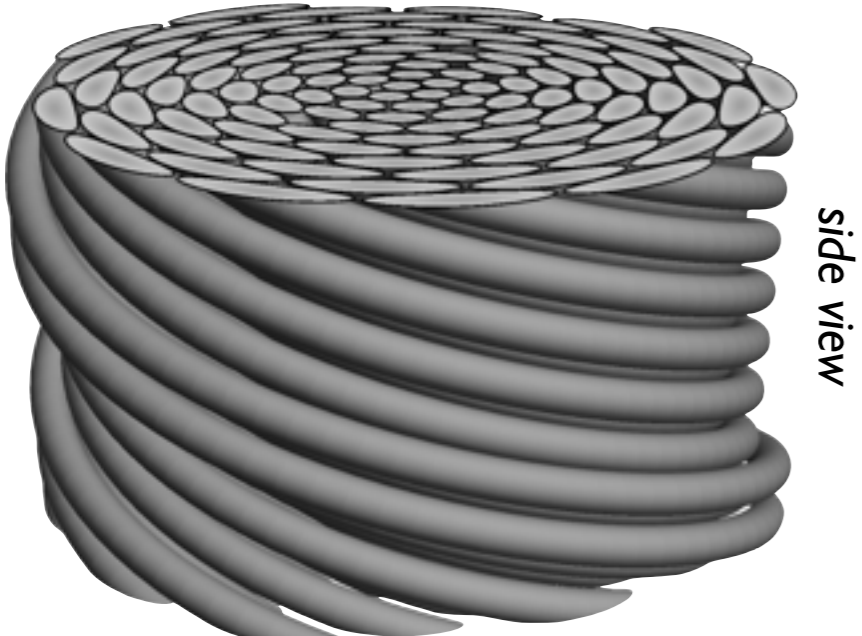
packing discs on sphere  
(orthographic projection)





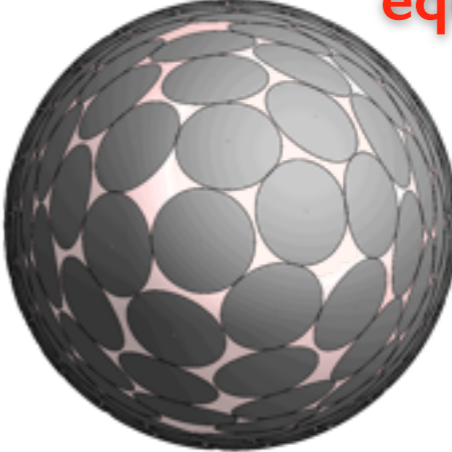
# Mapping frustration in filament packing

cross-section of twisted bundle

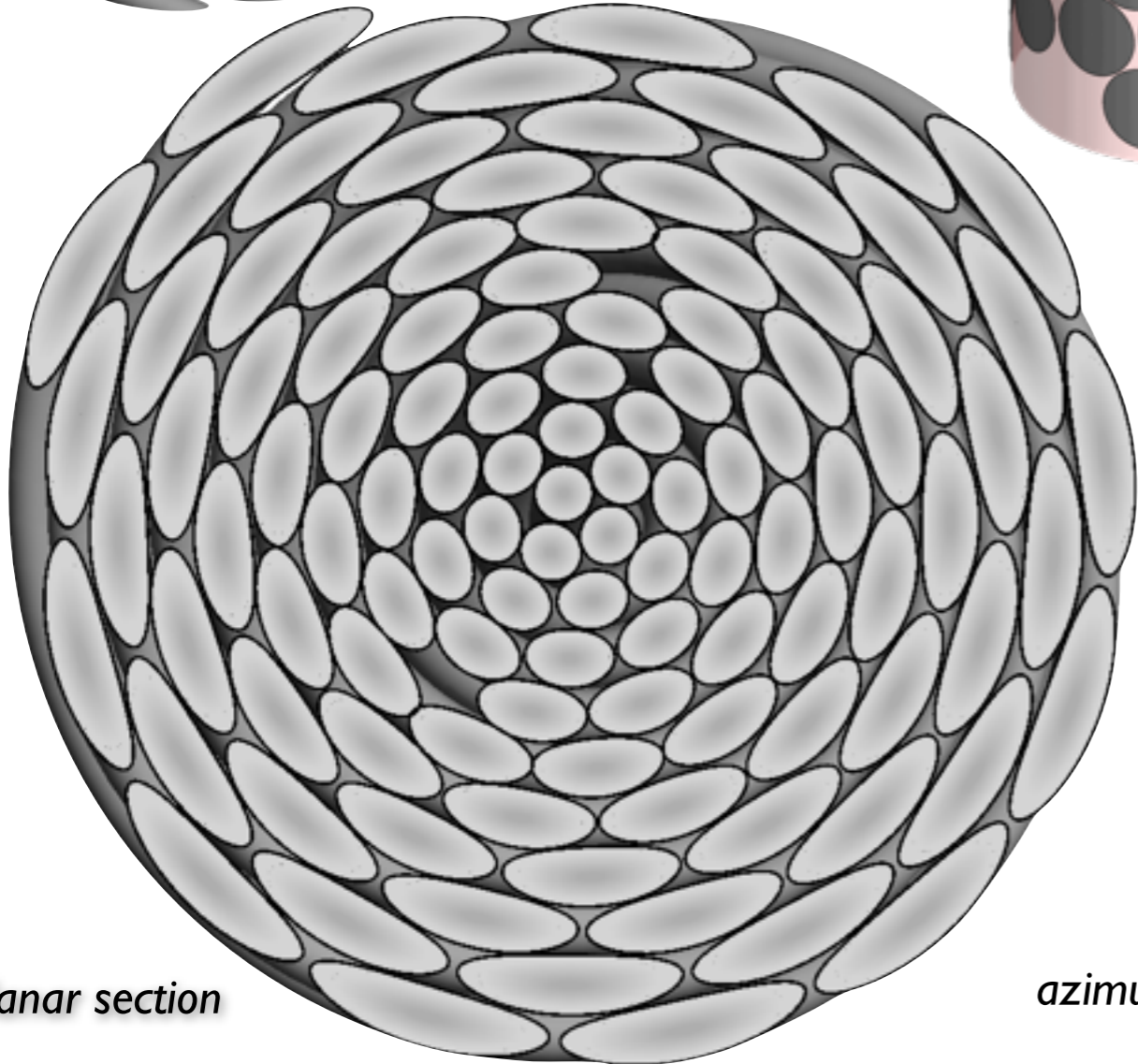


side view

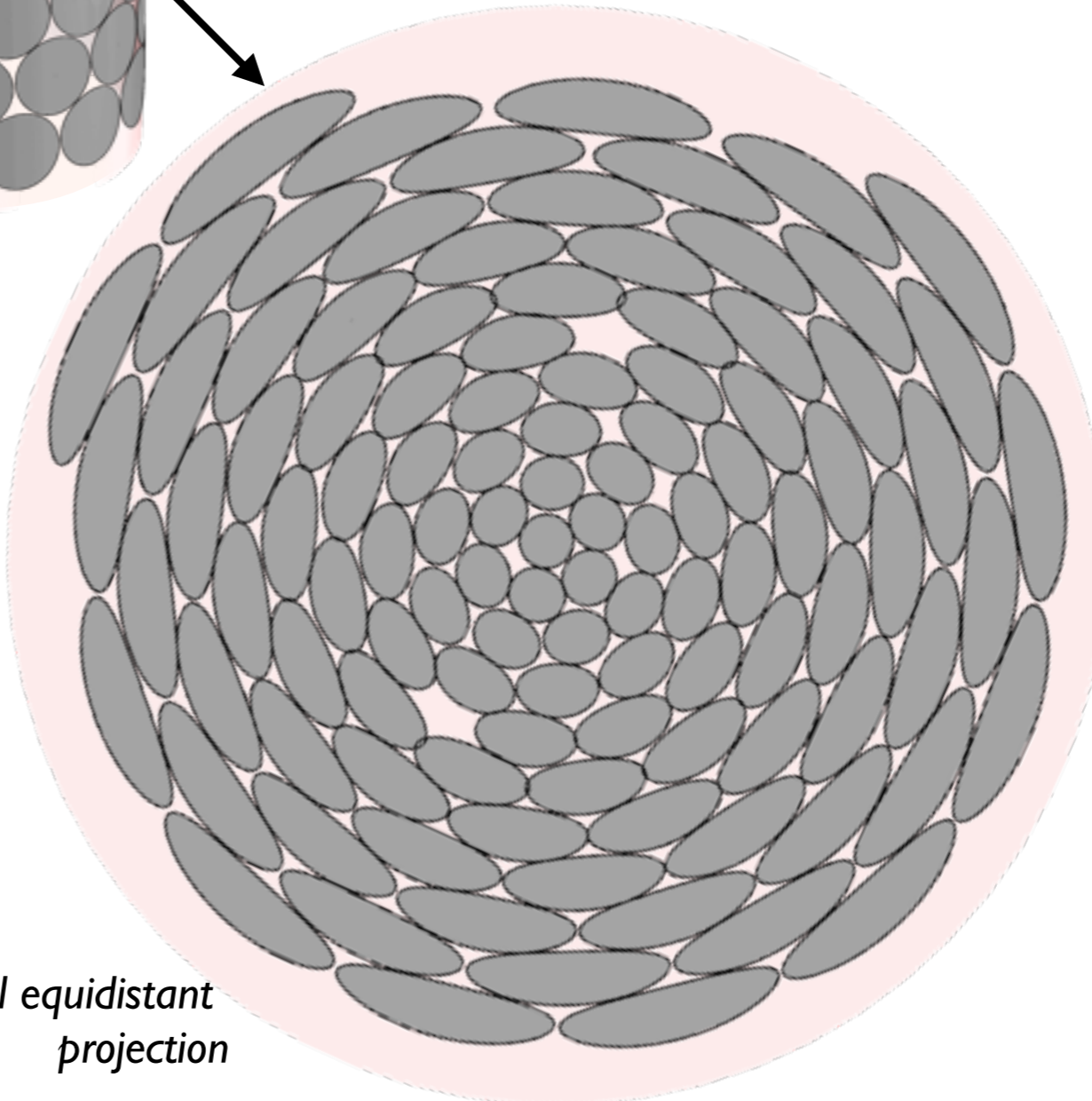
packing discs on a "bundle-equivalent dome"



orthographic projection ("from above")



planar section



azimuthal equidistant projection



# Geometric connection between filament arrays & 2D sheets

GMG, *Rev. Mod. Phys.* (2015).

infinitesimal filament spacing

in-place coords.

$$|d\Delta_{\perp}|^2 = g_{ij}(\mathbf{x}) dx_i dx_j$$

**inter-filament (2D) metric:**

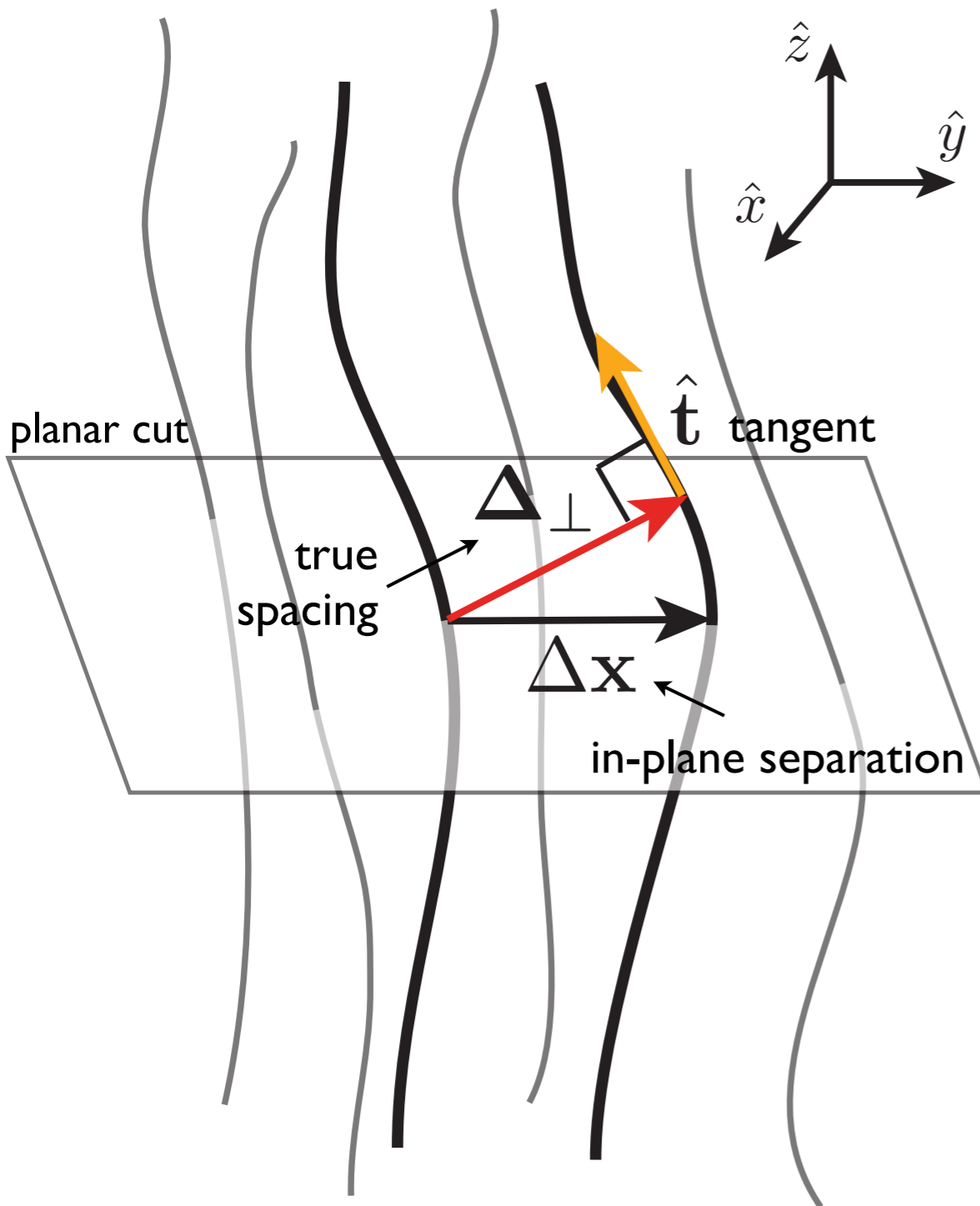
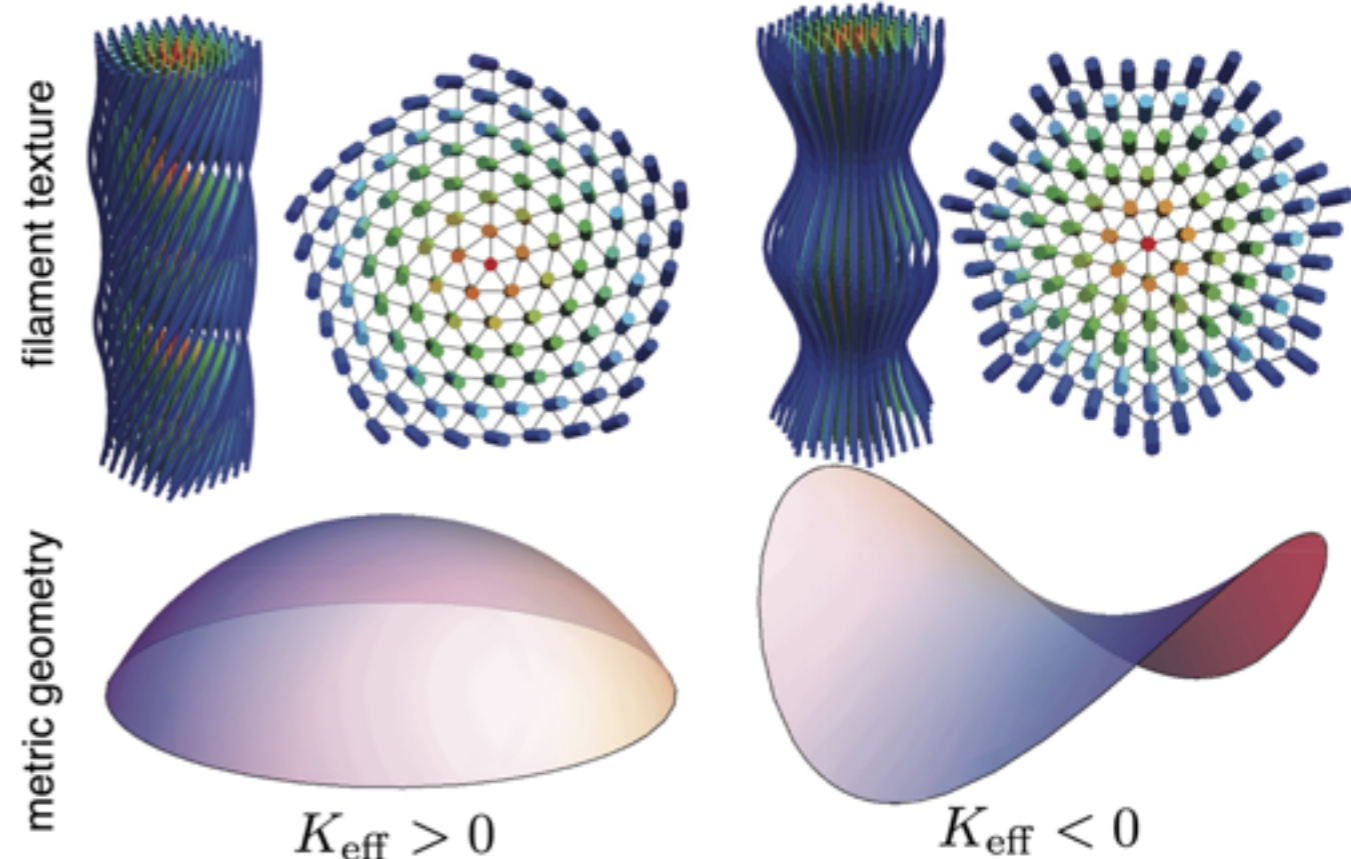
$$g_{ij}(\mathbf{x}) = \delta_{ij} - t_i(\mathbf{x})t_j(\mathbf{x})$$

**Gaussian curvature (filament metric):**

$$K_{\text{eff}} \simeq \frac{1}{2} (\partial_x^2 t_y^2 + \partial_y^2 t_x^2 - 2\partial_x \partial_y t_x t_y)$$

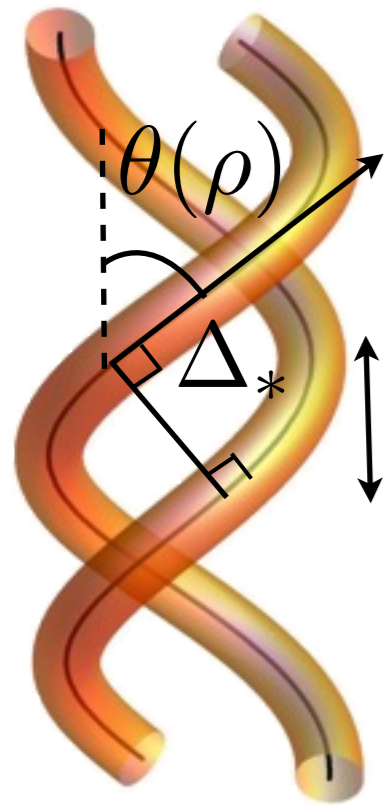
(double-)twist

splay





# Mapping frustration in filament packing



Distance of closest approach:  $\Delta_* = \min_z [\Delta(z)]$

Tilt angle (local):  $\sin \theta(\rho) = \frac{\Omega \rho}{\sqrt{1 + (\Omega \rho)^2}}$

Distance between helical curves:

$$\Delta^2(z) = \rho_1^2 + \rho_2^2 - 2\rho_1\rho_2 \cos(\Omega z + \phi_1 - \phi_2) + z^2$$

Metric geometry of bundles:

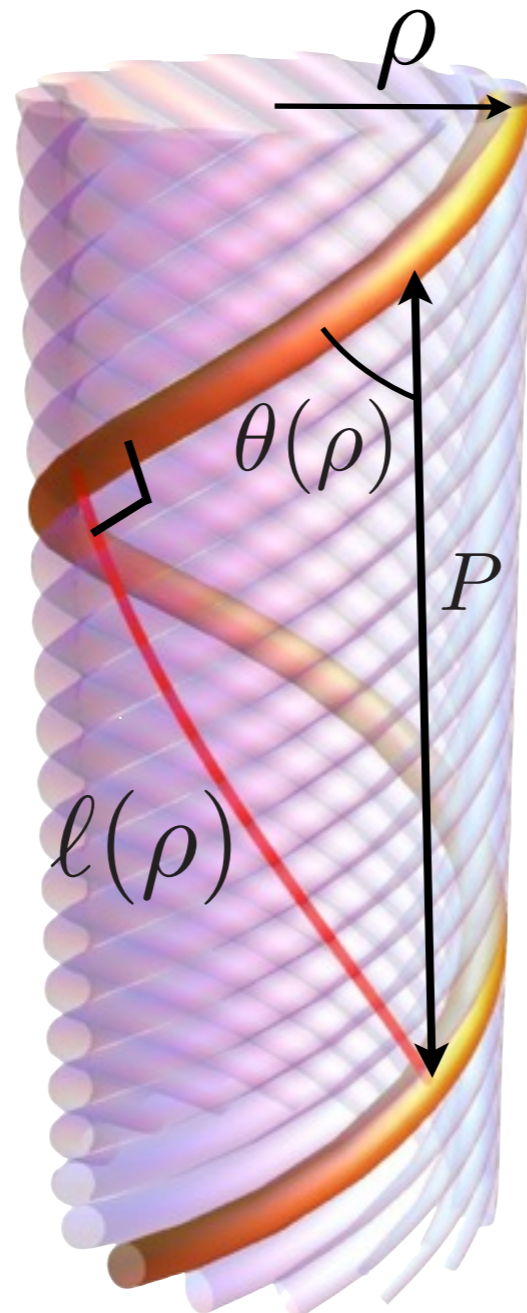
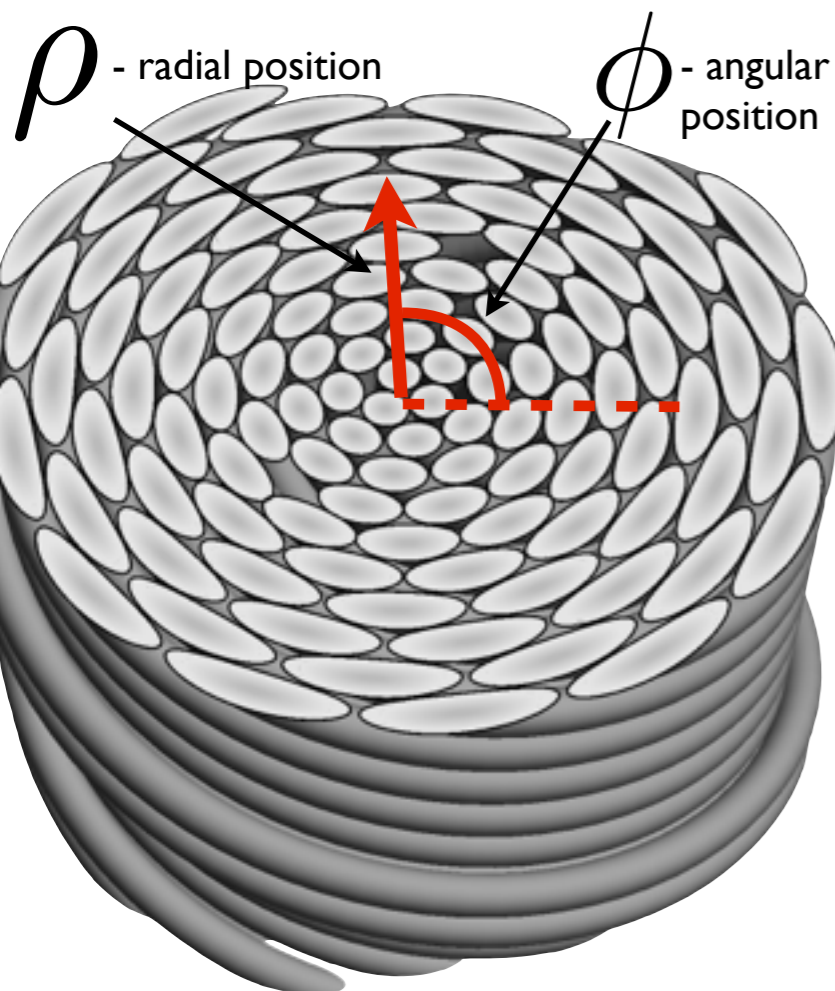
$$\lim_{\delta\phi \rightarrow 0, \delta\rho \rightarrow 0} \Delta_*^2 \equiv ds^2 = (\delta\rho)^2 + \Omega^{-2} \sin^2 \theta(\rho) (\delta\phi)^2$$

**Perimeter:** space available in bundle @  $\rho$

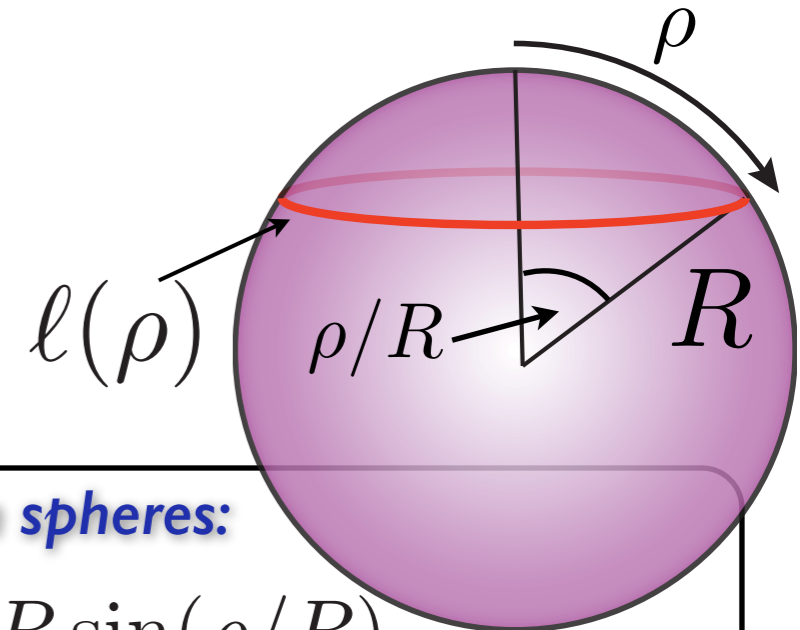
$$\ell(\rho) = P \sin \theta(\rho)$$

less than planar packing!

$$\simeq 2\pi\rho \left(1 - \frac{\Omega^2}{2} \rho^2\right)$$



$$P = \frac{2\pi}{\Omega}$$



**Latitudes on spheres:**

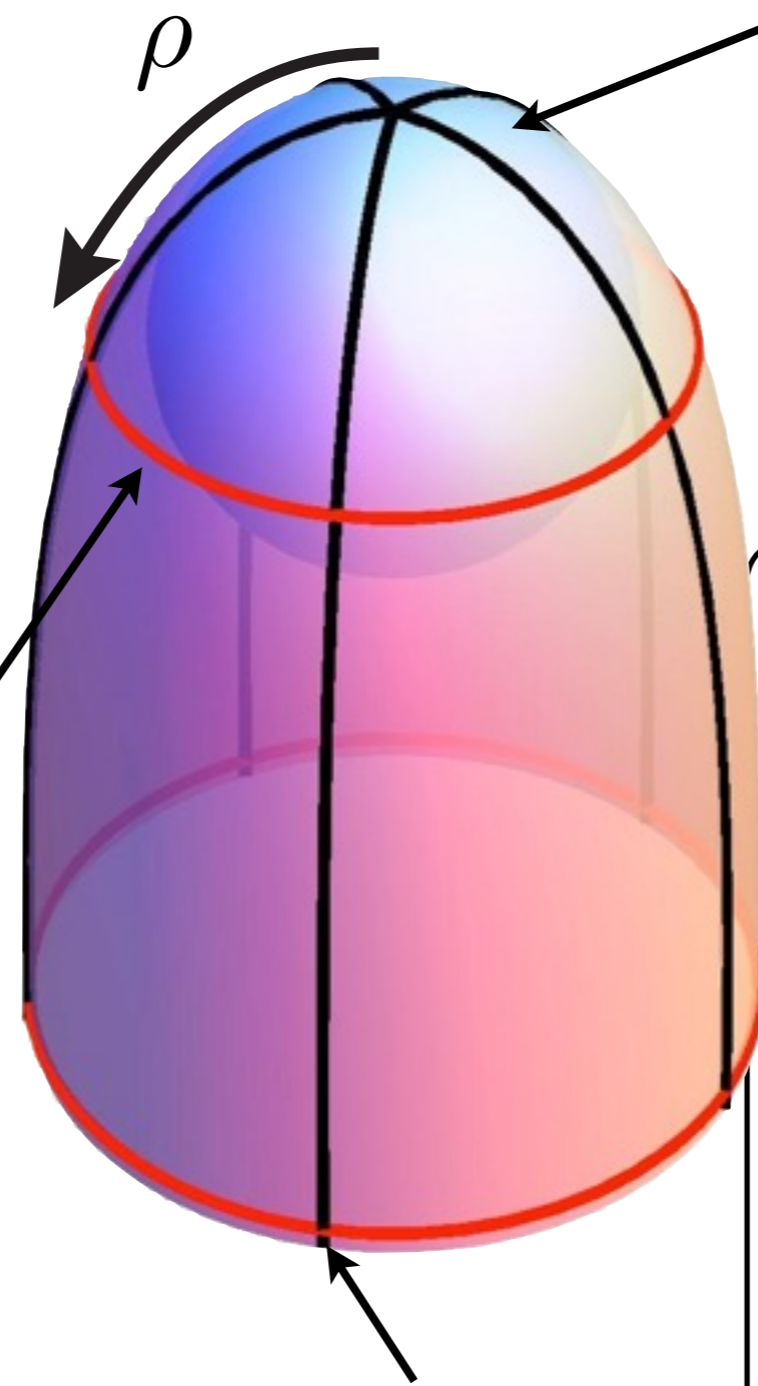
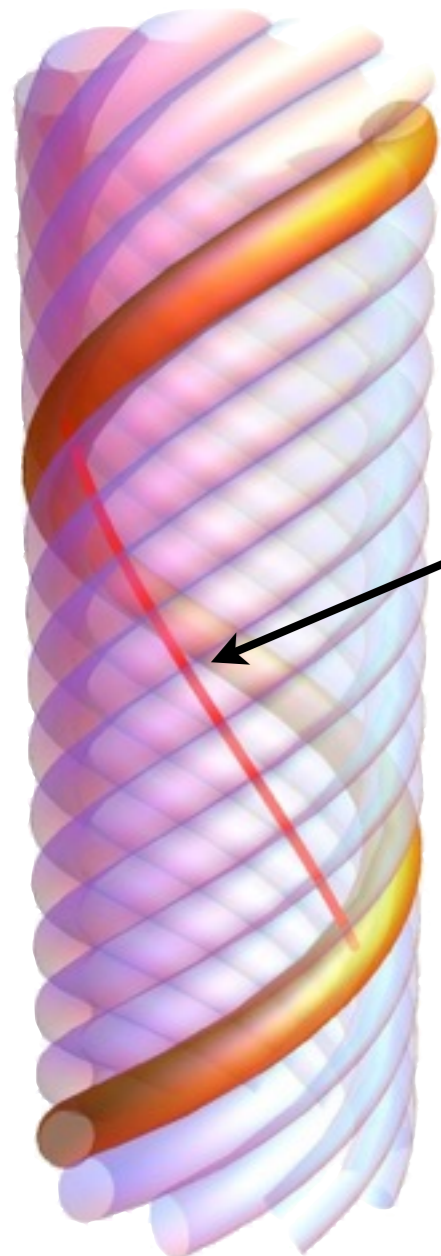
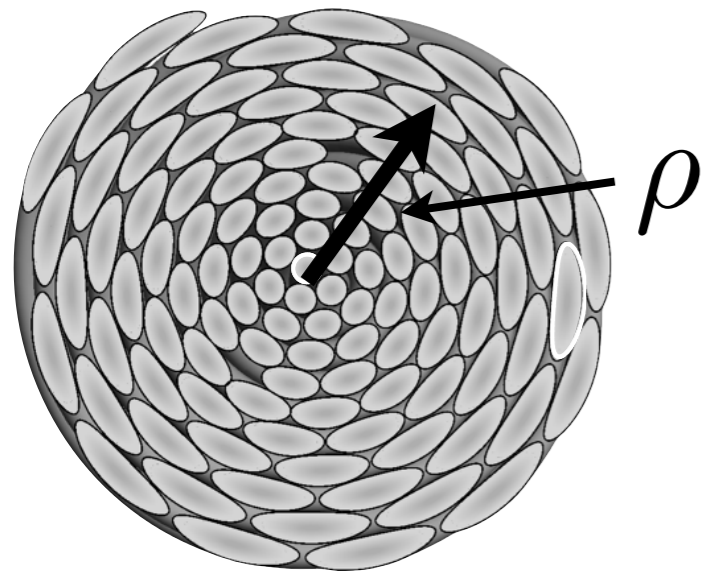
$$\ell(\rho) = 2\pi R \sin(\rho/R)$$

$$\simeq 2\pi\rho \left(1 - \frac{1}{6R^2} \rho^2\right)$$



# Frustration in filament packing: hidden geometry

**Twisted bundle packing is equivalent to packing on curved surface!**



spherical radius =  $\frac{\Omega^{-1}}{\sqrt{3}}$

$$K_G = -\frac{3\Omega^2}{[1 + (\Omega\rho)^2]^2}$$

Gaussian curvature of "dual surface" to twisted filament bundle

$K_G = \kappa_1 \kappa_2$

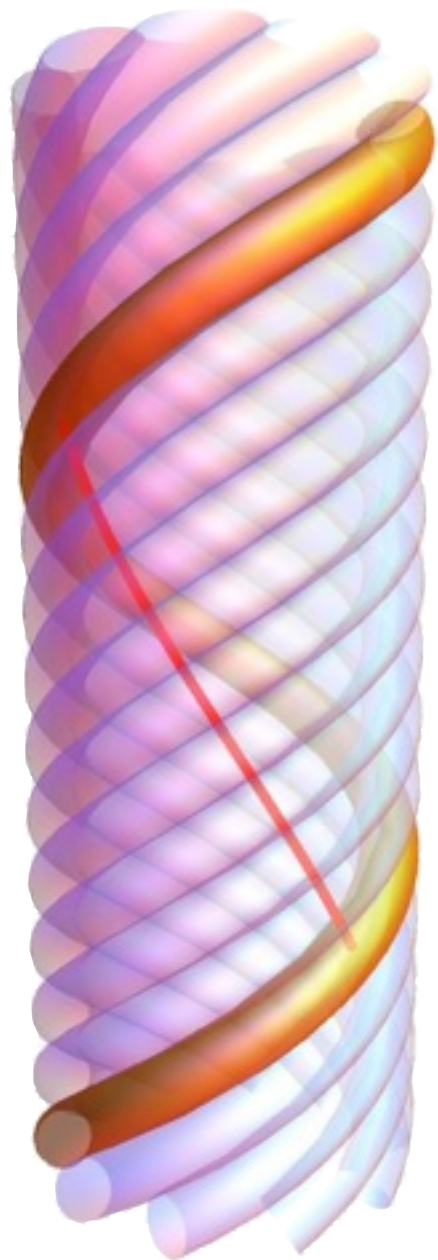
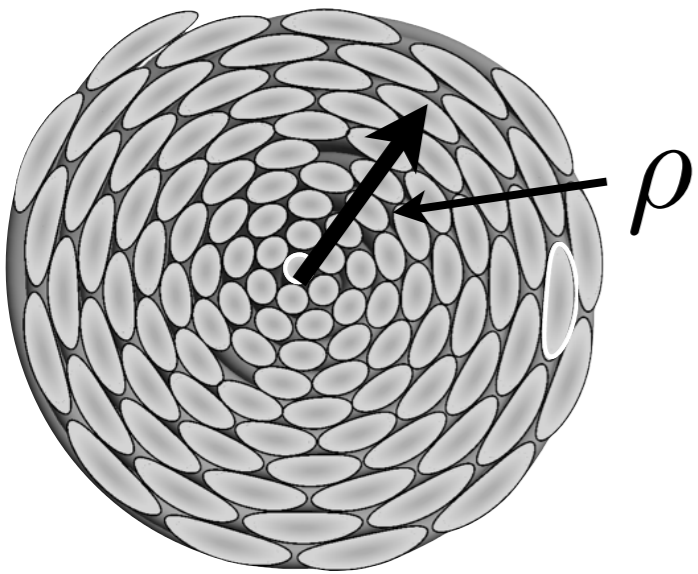
$K_G < 0$        $K_G > 0$

The complex block contains a diagram illustrating the Gaussian curvature  $K_G = \kappa_1 \kappa_2$ . It shows two overlapping curved surfaces, one orange and one purple, with principal curvatures  $\kappa_1^{-1}$  and  $\kappa_2^{-1}$  indicated. To the right is a spherical cap with a grid of lines. Below the diagram, the text  $K_G < 0$  and  $K_G > 0$  is shown.

cylindrical radius =  $\Omega^{-1}$

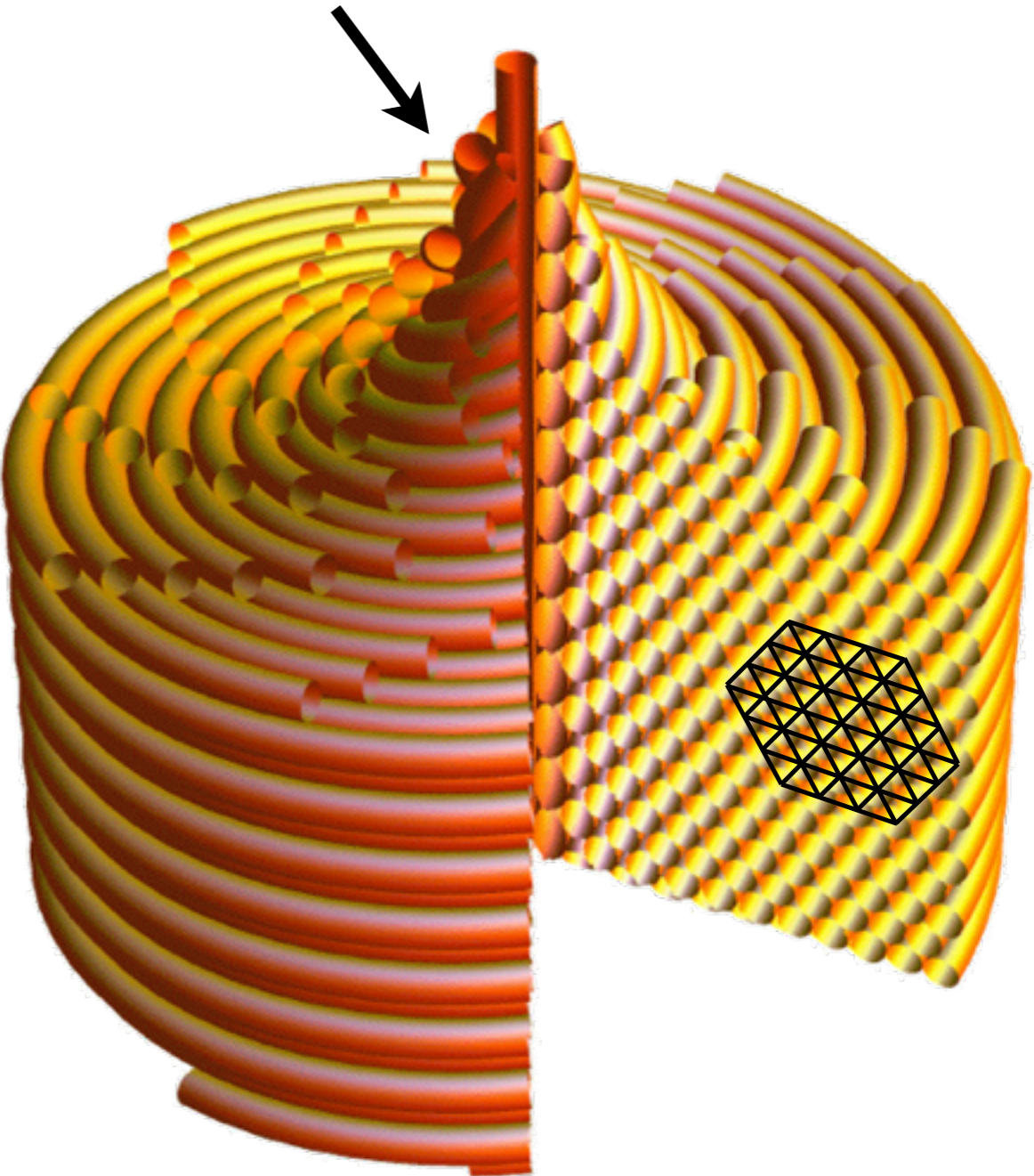


# Frustration in filament packing: hidden geometry



Perfect, regular packing is **frustrated** (disrupted) at the central core of twisted bundles

=



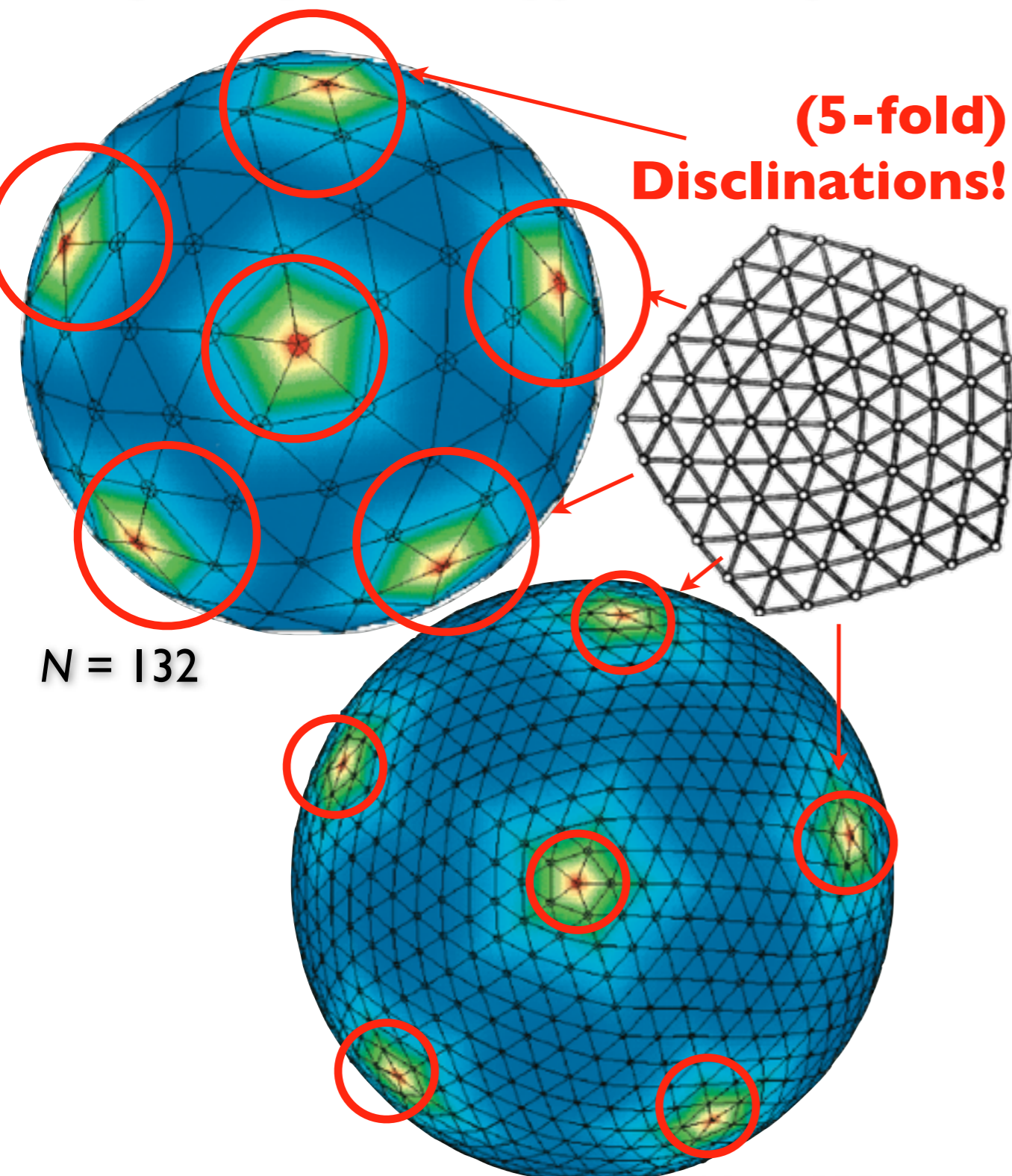
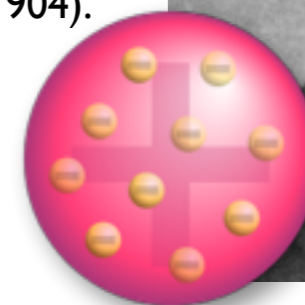


# Spherical Crystallography: Generalized Thomson Problem

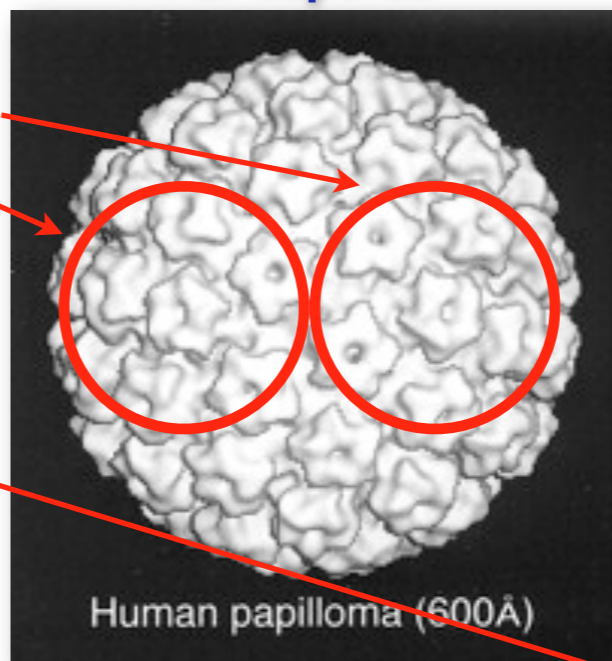
Repulsive (electrostatic) particles on spheres

“plum pudding”  
model:

electronic “corpuscles”  
on a charged sphere  
Thomson, *Phil. Mag.* (1904).

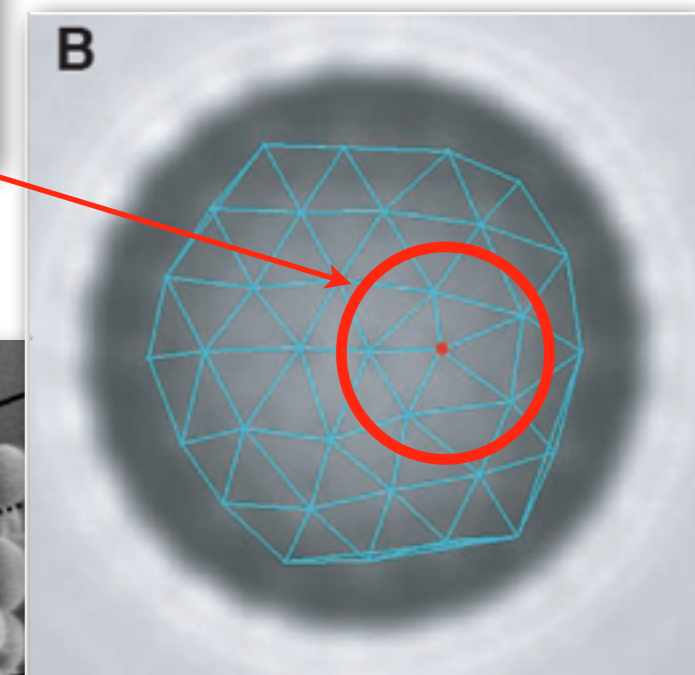


Viral capsids

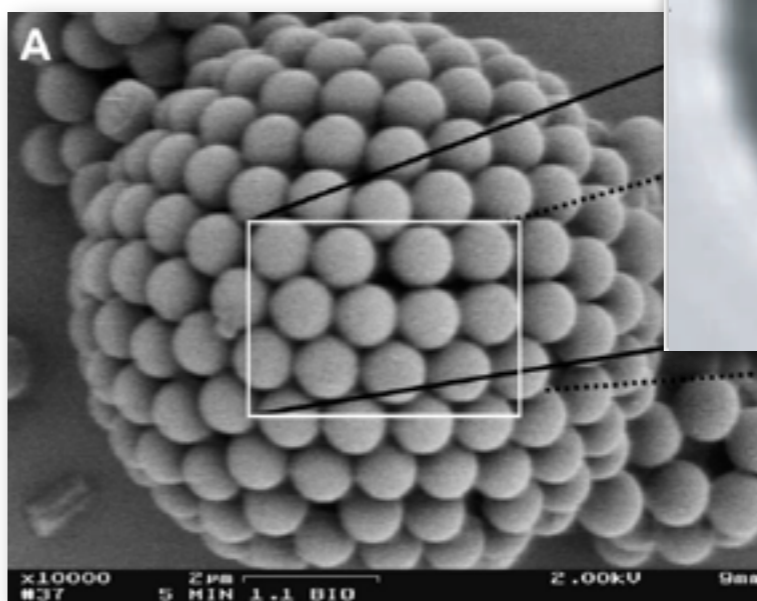


Baker, Oslen & Fuller,  
*Micro. & Mol. Biol. Rev.* (1994).

Colloidsomes



Bausch, Bowick, Cacciuto, Dinsmore,  
Hsu, Nelson, Nikolaides, Travesset &  
Weitz, *Science* (2003)



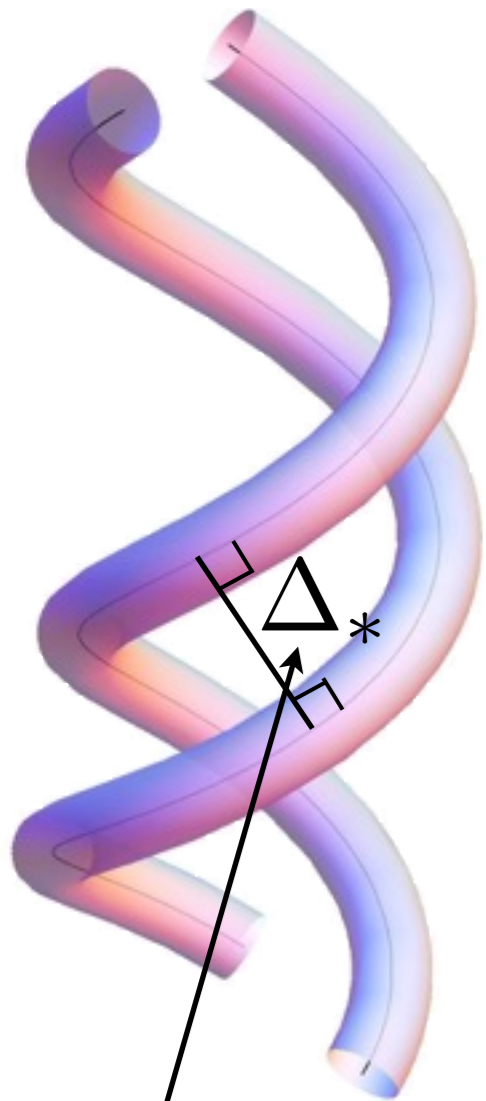
Dinsmore, Hsu, Nikolaides, Marquez  
& Weitz, *Science* (2002)

Altschuler, Williams, Ratner, Tipton, Stong,  
Dowla & Wooten, *Phys Rev Lett* (1999)

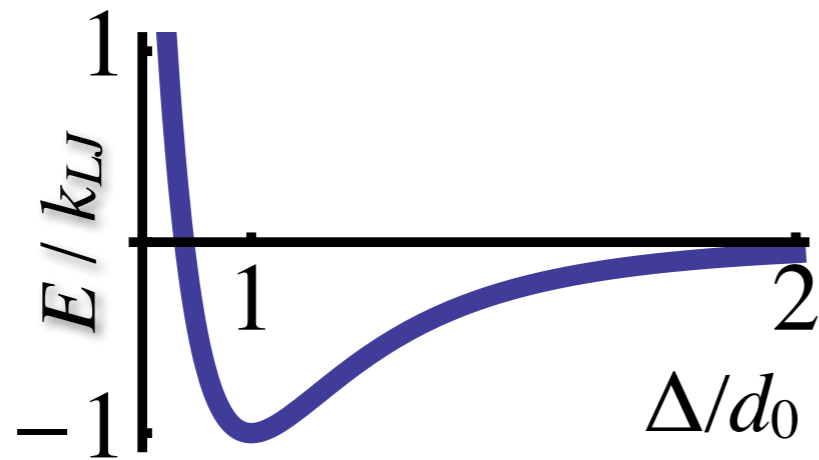


# Simulations of adhesive filament, twisted assemblies

Method: (numerically) minimize 2D cross-section of  $N$  filament bundles of fixed twist interacting via attractive, pair-wise forces



$$E_{LJ} = \frac{k_{LJ}}{2} \left( \frac{5d_o^{12}}{6\Delta^{11}} - \frac{11d_o^6}{6\Delta^5} \right)$$

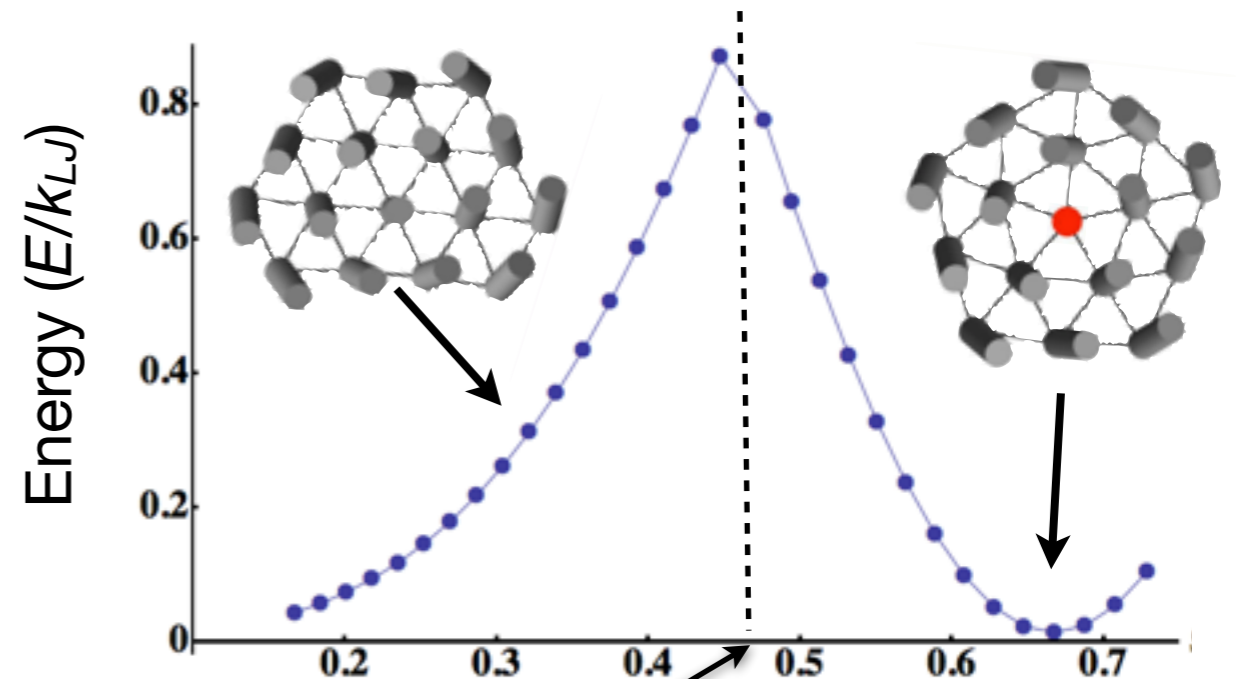


Pair-wise adhesive energy ("Curva-Lennard Jones")

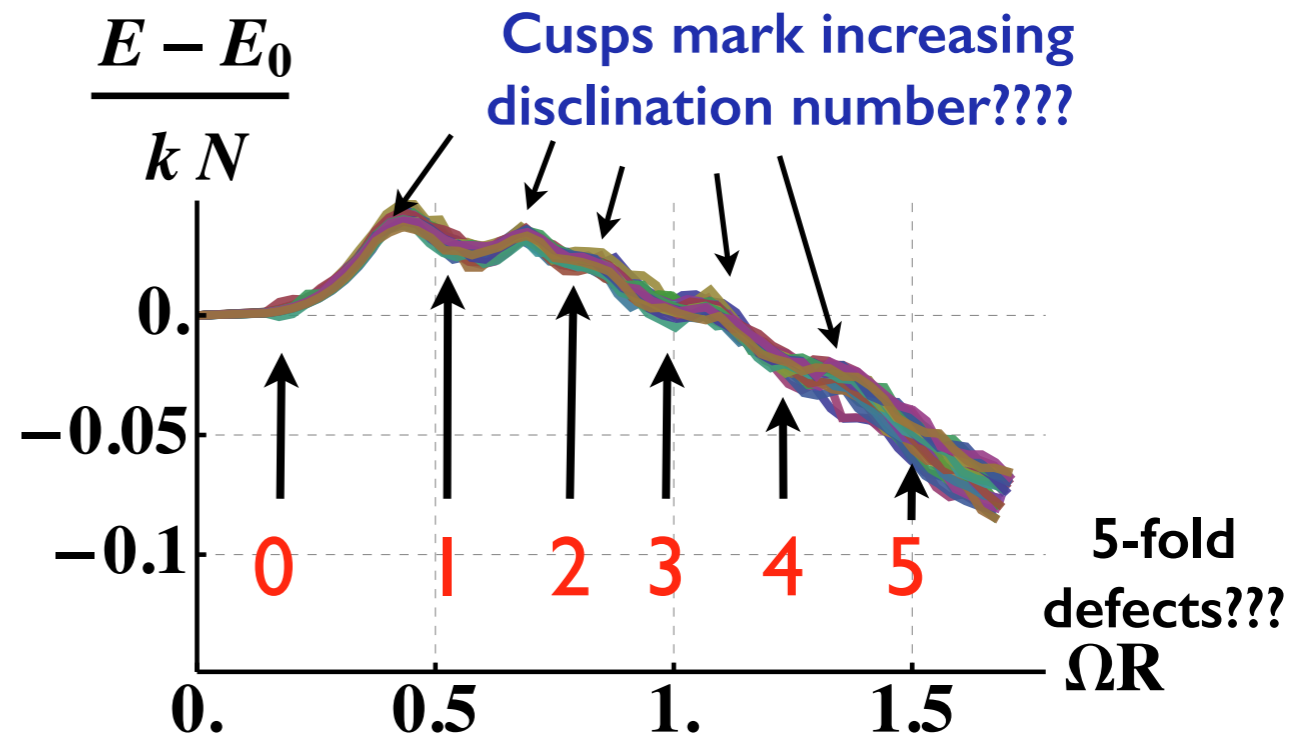
$N = 85 - 154$   
filaments

## 16 filament bundle

small twist (no defect)

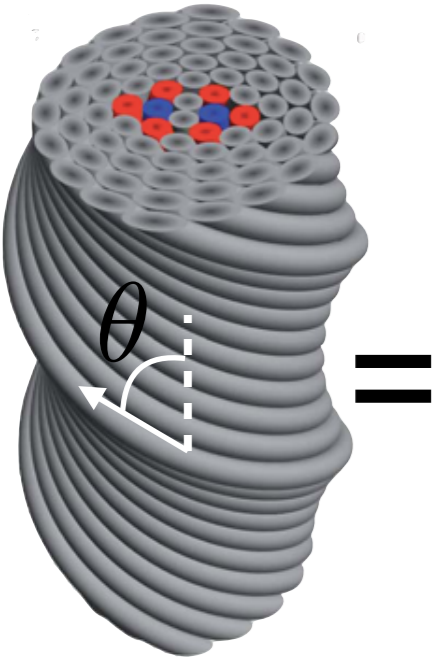


$|\Omega R|_c \simeq 0.471$  ( $\Omega R$ ) - bundle twist

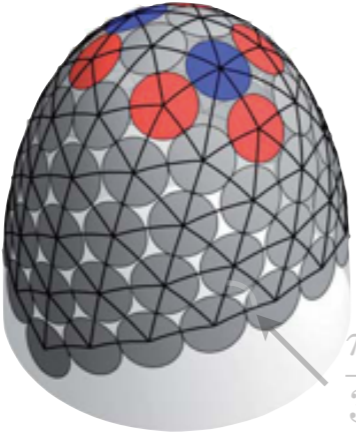




# Defects in Ground States of Small-N Bundles



=



**Total disclination “charge” (# 5’s - #7’s):**

$$Q = \sum_n (n - 6) V_n$$

# of  $n$ -fold coordinated filaments

$\frac{\pi}{3} + \Delta\theta_b$   
“equilateral excess”

**Generalized Euler-Poincare formula (triangulation w/open boundary):**

$$6 \int dA K_G = 2\pi Q + \sum_b \Delta\theta_b$$

~~distortion @ boundary~~

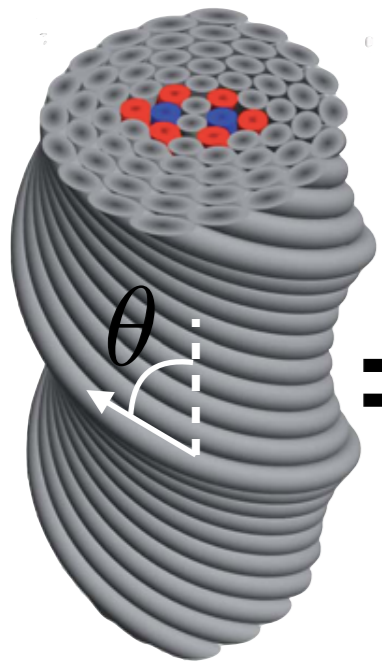
**“Net neutral” disclination charge:**

$$Q_{id} = \frac{3}{\pi} \int dA K_{eff} = 6(1 - \cos^3 \theta)$$

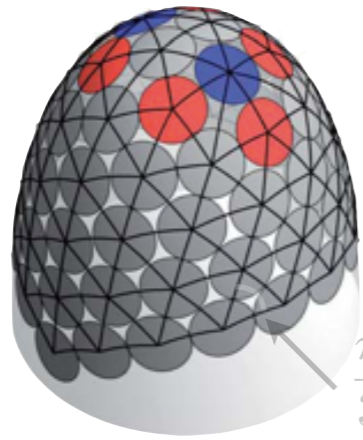
bundle twist angle



# Defects in Ground States of Small- $N$ Bundles



=



Total disclination "charge"  
(# 5's - #7's):

$$Q = \sum_n (n - 6) V_n$$

# of  $n$ -fold coordinated filaments

$$\frac{\pi}{3} + \Delta\theta_b$$

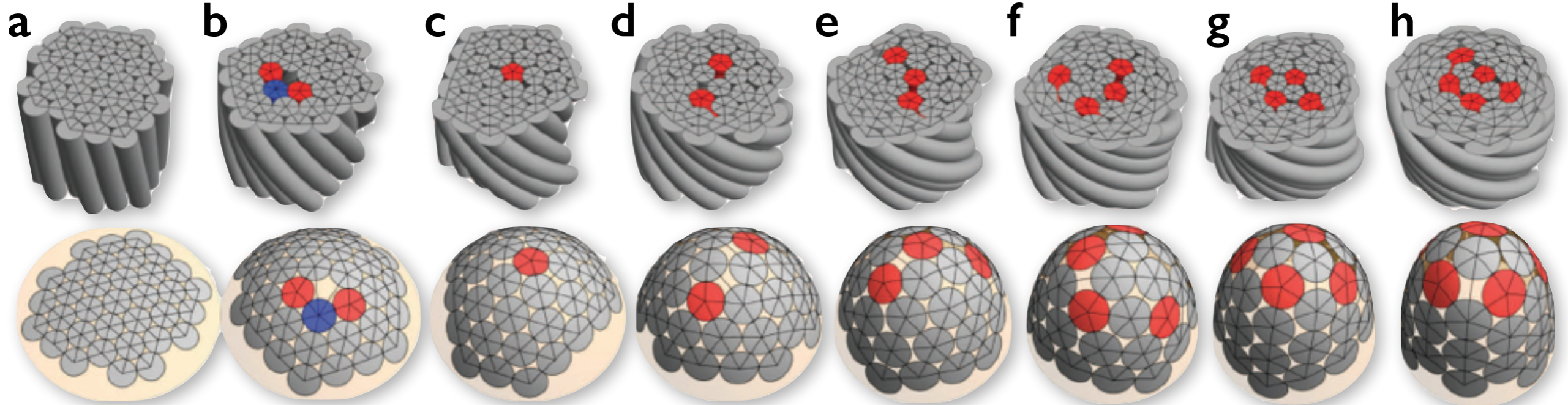
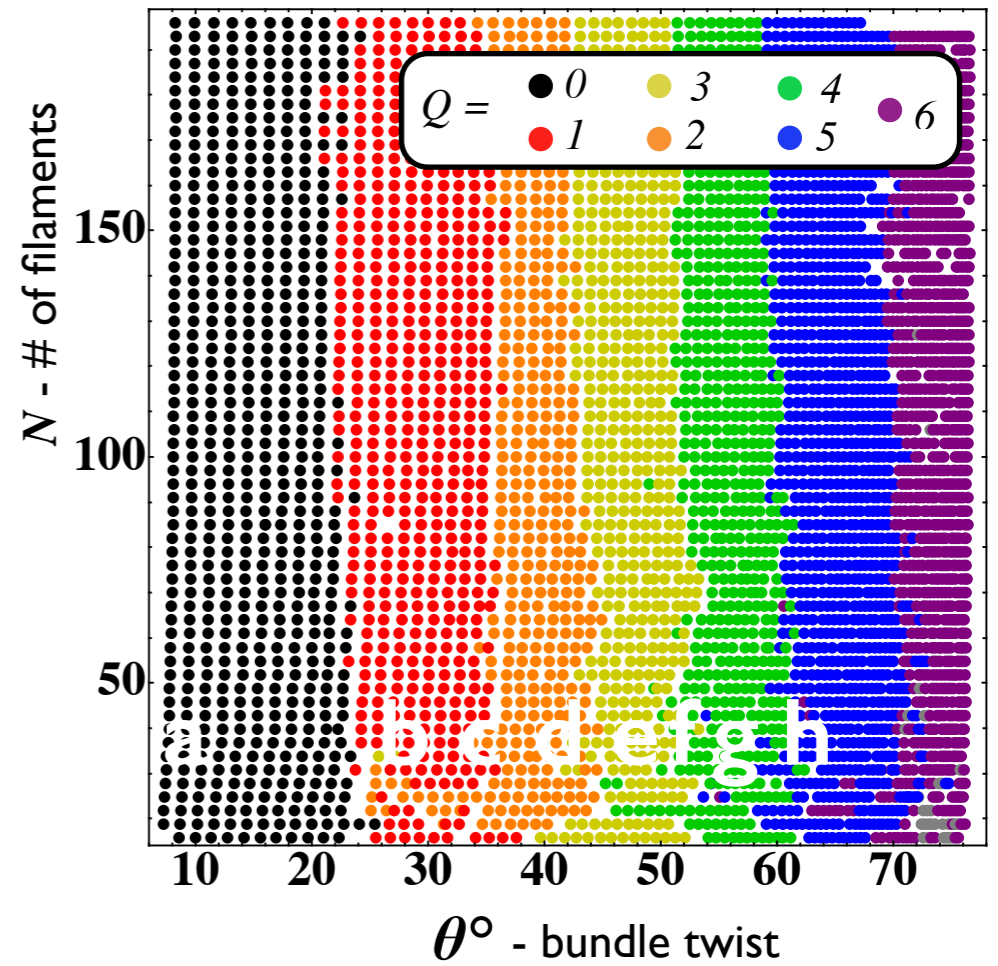
"equilateral excess"

"Net neutral" disclination charge:

$$Q_{id} = \frac{3}{\pi} \int dA K_{\text{eff}} = 6(1 - \cos^3 \theta)$$

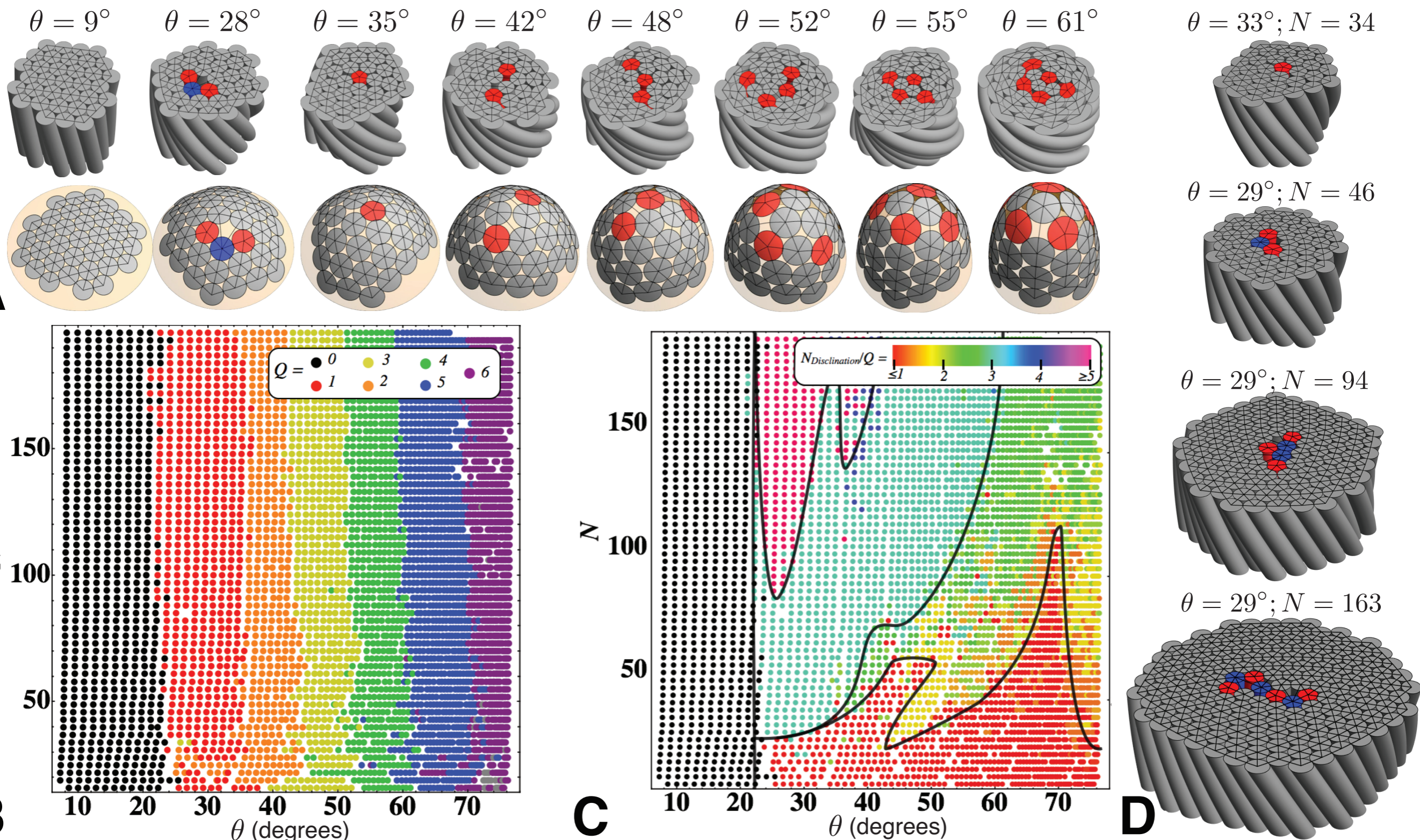
bundle twist angle

ground state defect charge,  $Q$



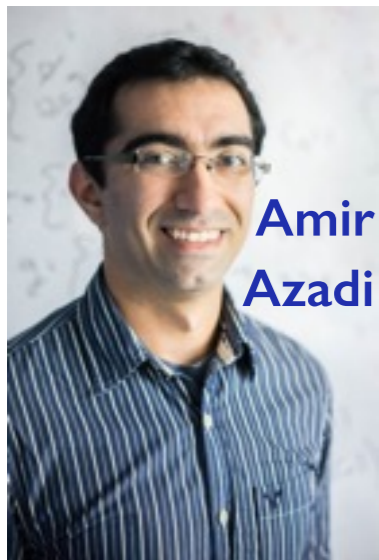


# Numerical “ground states” of small- $N$ bundles:



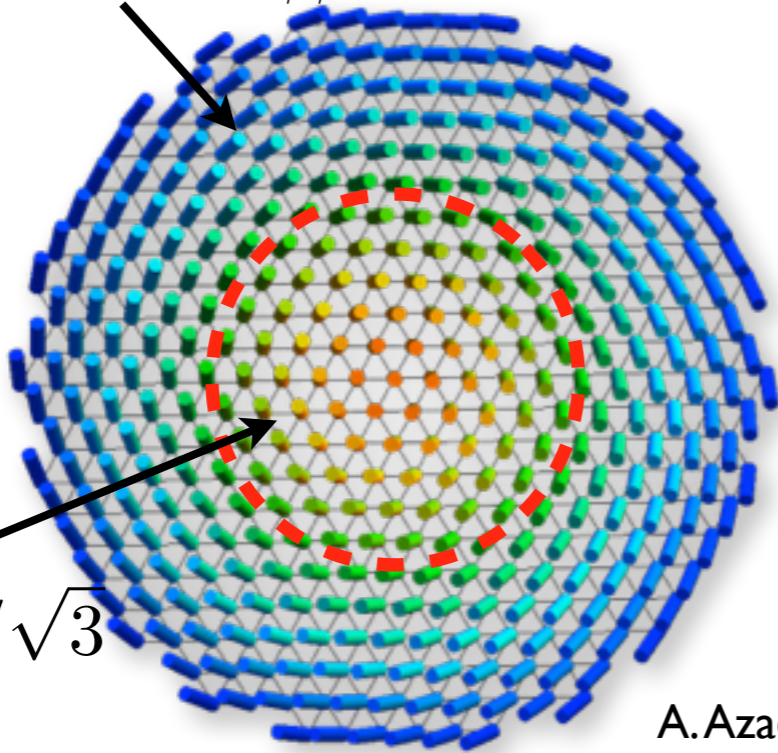


# Large- $N$ Bundles: Multi-dislocation ground states



twist-induced stresses:

compression:  $\sigma_{\phi\phi} < 0; \rho > R/\sqrt{3}$

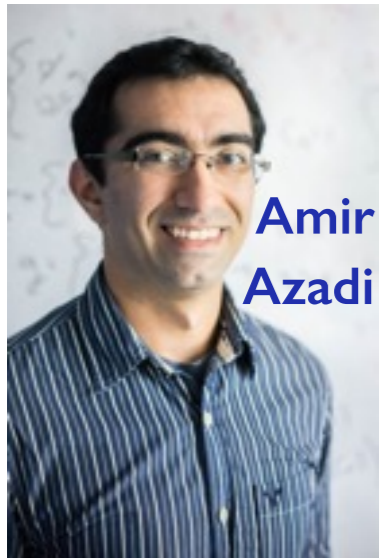


tension:  $\sigma_{\phi\phi} > 0; \rho < R/\sqrt{3}$

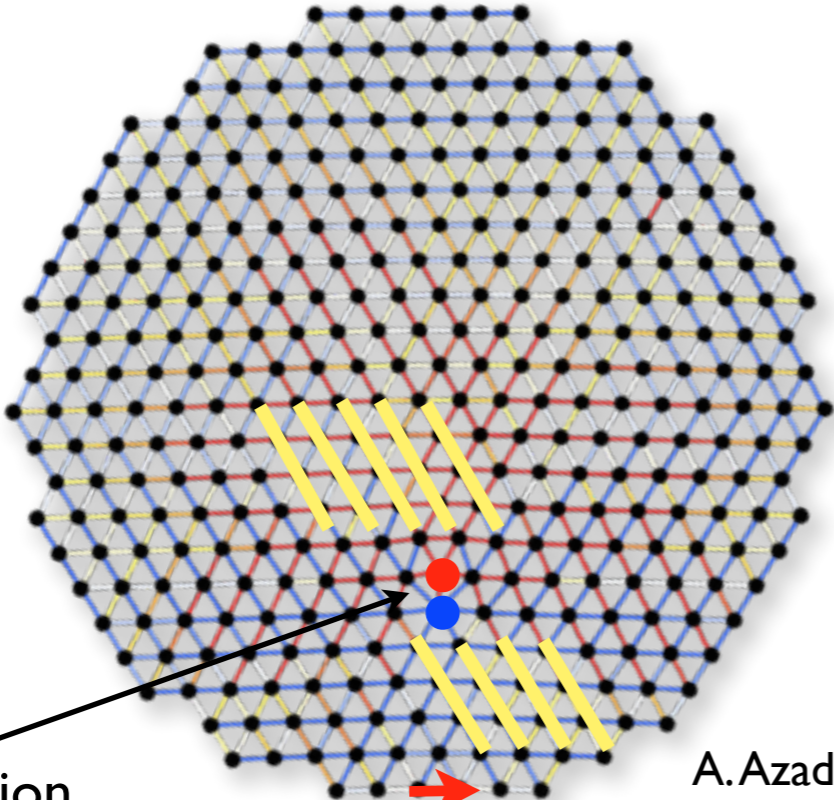
A.Azadi & GMG, PRE (2012).



# Large- $N$ Bundles: Multi-dislocation ground states



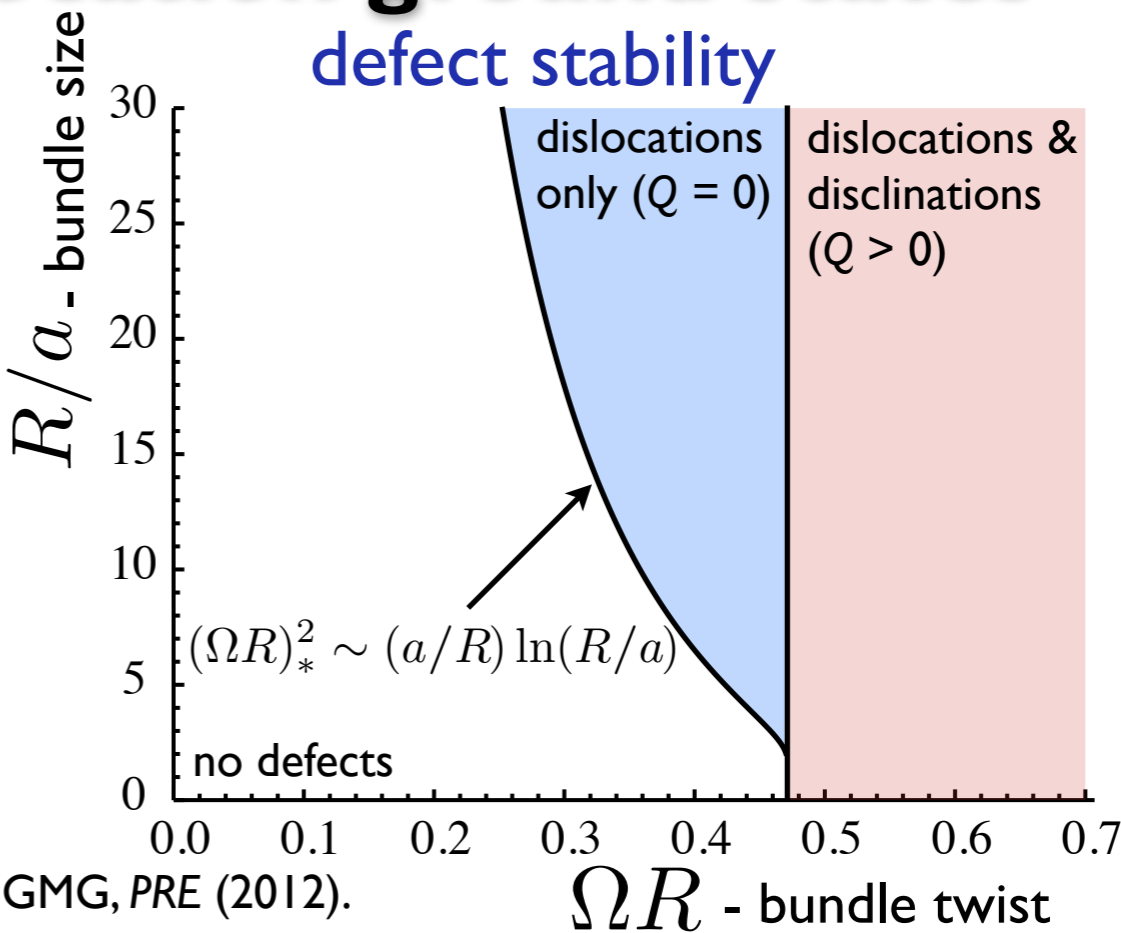
Amir Azadi



edge dislocation (5-7 pair)

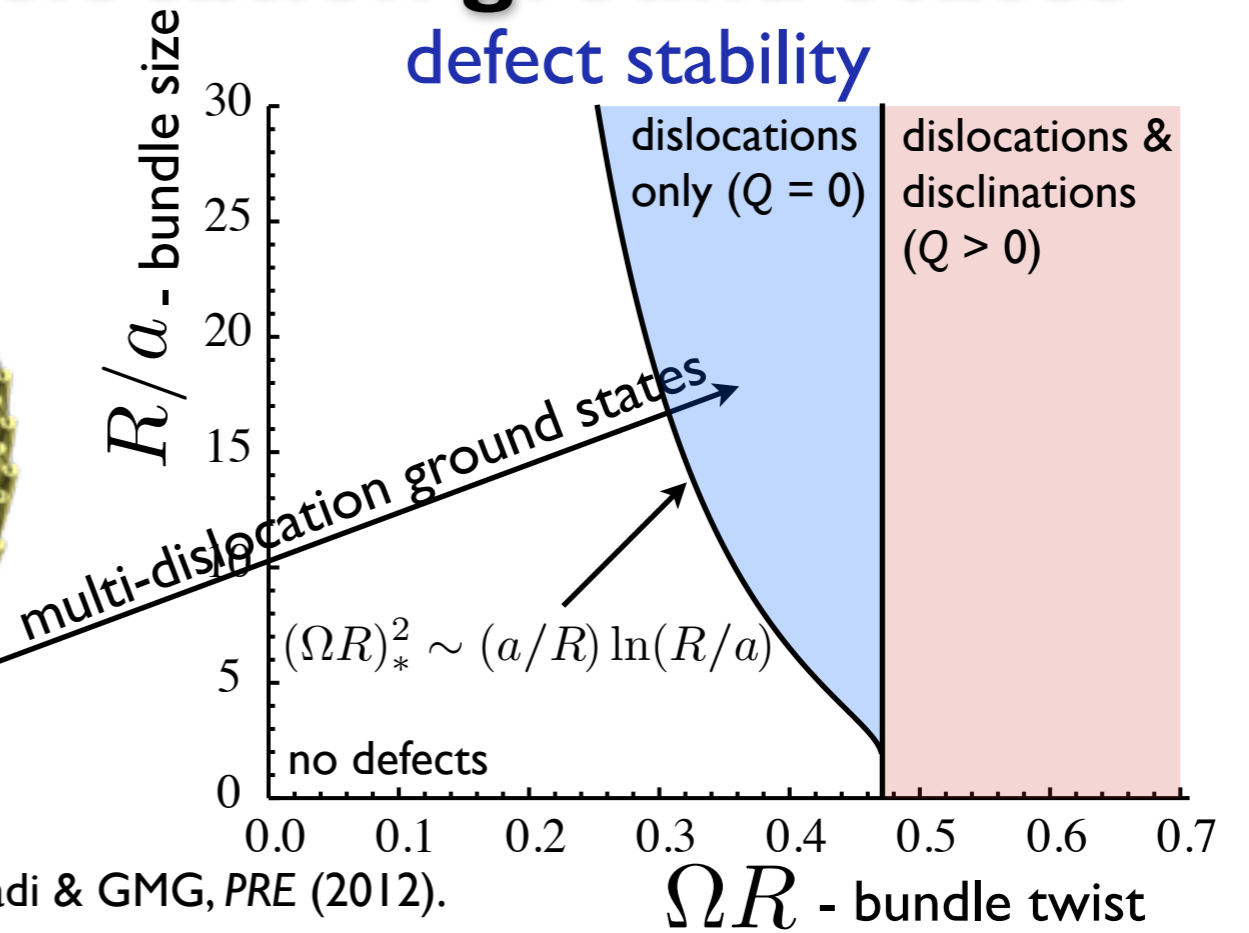
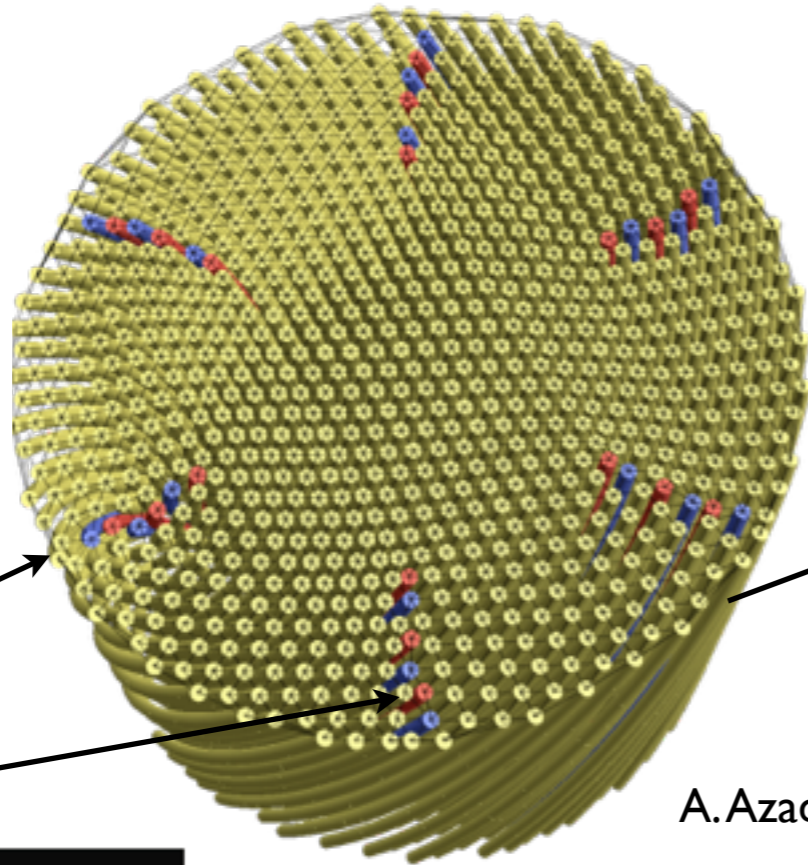
**b** - Burger's vector

A. Azadi & GMG, *PRE* (2012).

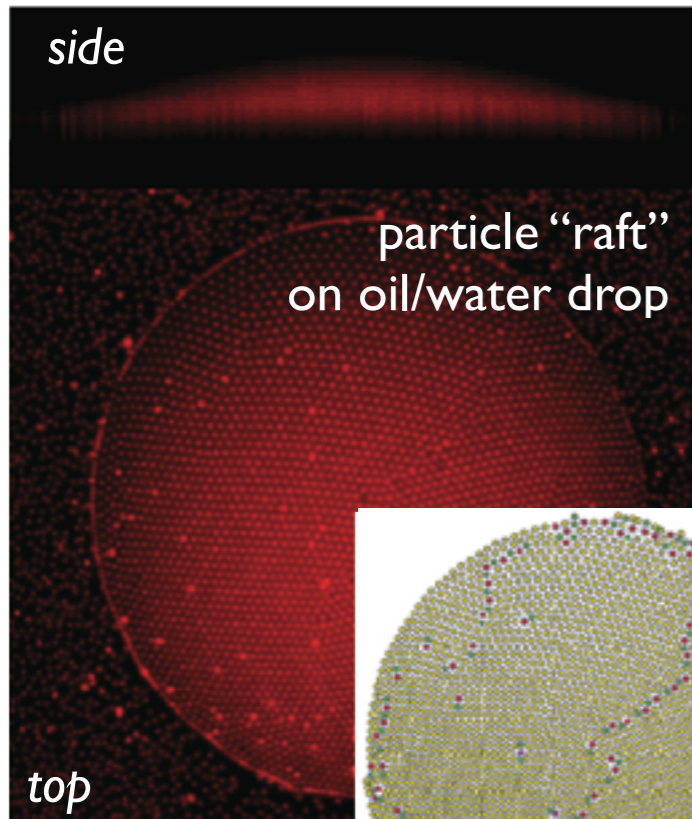




# Large- $N$ Bundles: Multi-dislocation ground states



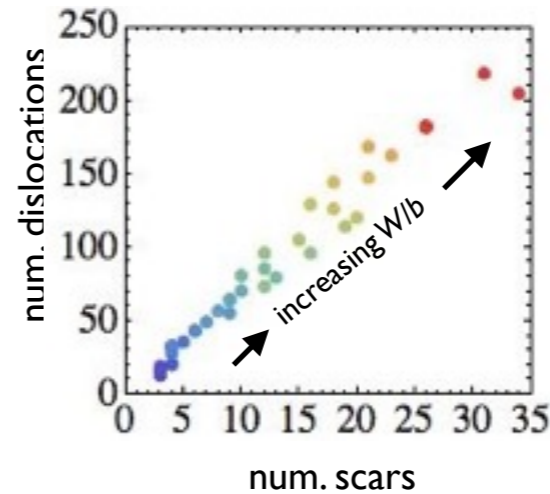
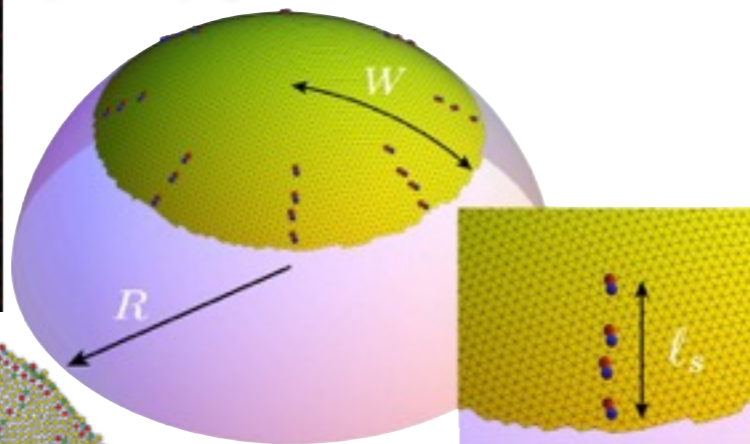
A. Azadi & GMG, *PRE* (2012).



Irvine @ U Chicago

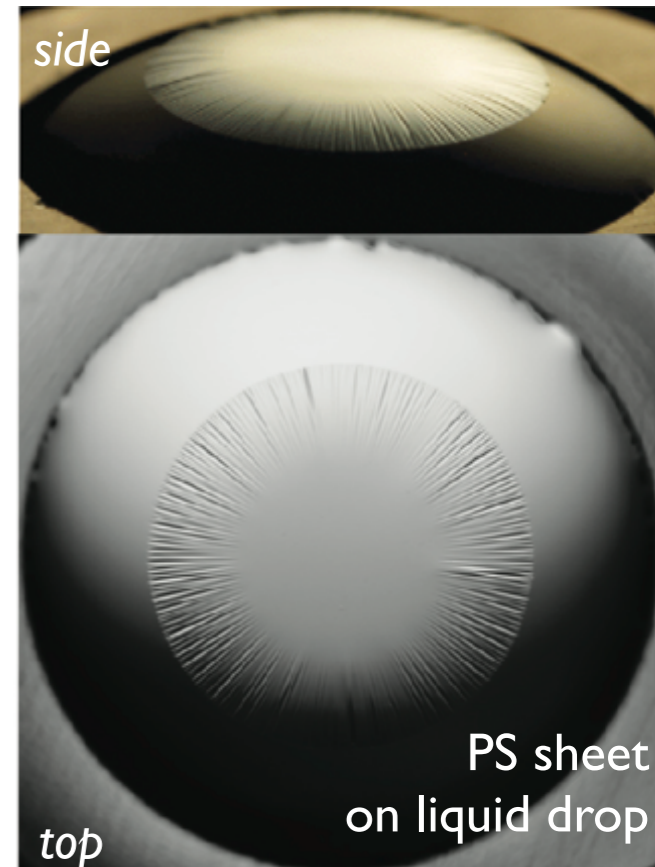
## Optimal symmetry of multi-dislocation (scar) patterns?

A. Azadi & GMG, *PRL* (2014).



## Ground states of surface confined assemblies: "elastic" wrinkle vs. "plastic" defect patterns?

GMG & Davidovitch, *PNAS* (2013).

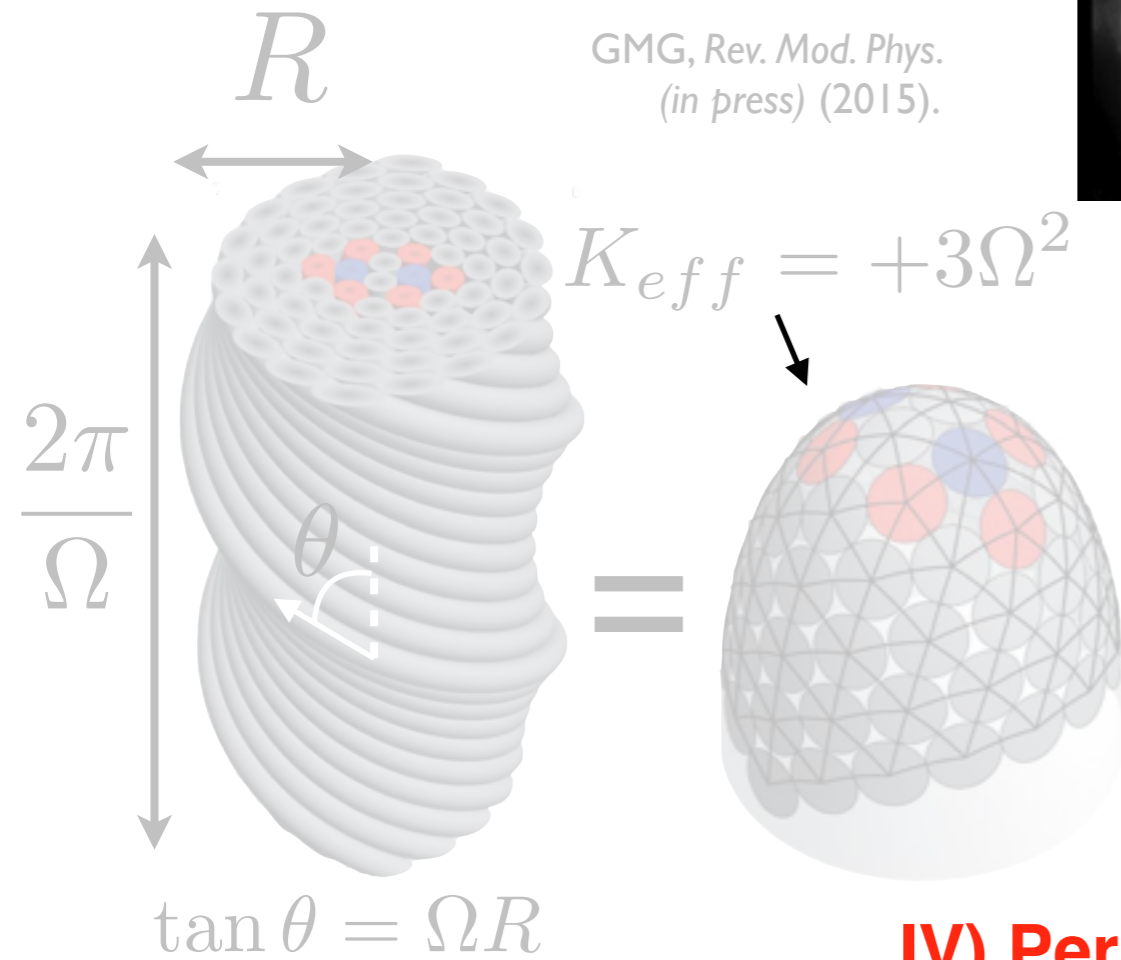


Menon @ UMass

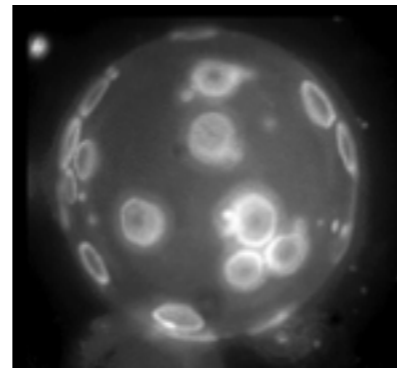


# Twisted bundles: non-Euclidean geometry & anomalous assembly

## I) Non-euclidean metric geometry of bundles

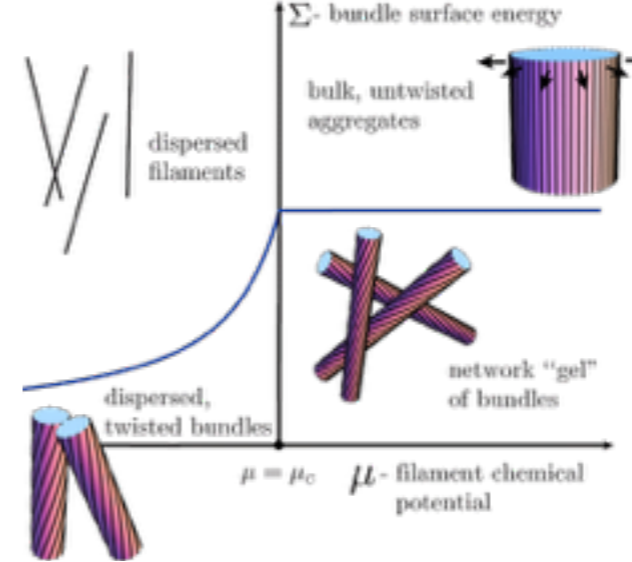


## solid domains on lipid vesicles



Bandekar & Sofou, *Langmuir* (2012)

## chiral filament assembly



## II) Self-limiting Assembly

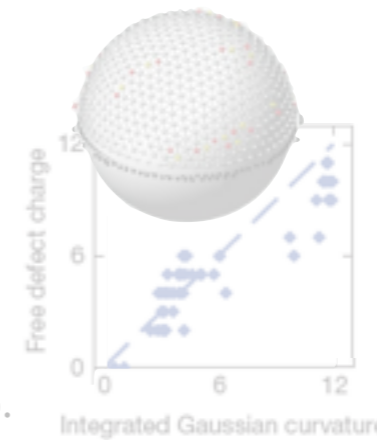
GMG & Bruinsma, *PRL* (2007); GMG, *PRE* (2009)

## III) Topological Defects

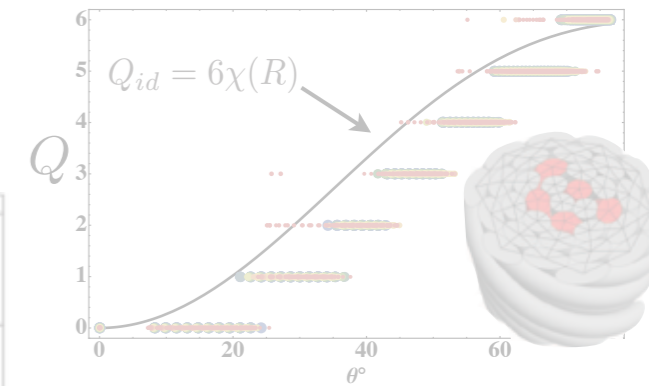
defects in curved crystals



Irvine et al., *Nature* (2010).



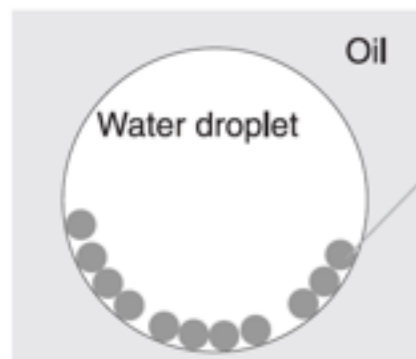
defects in twisted bundles



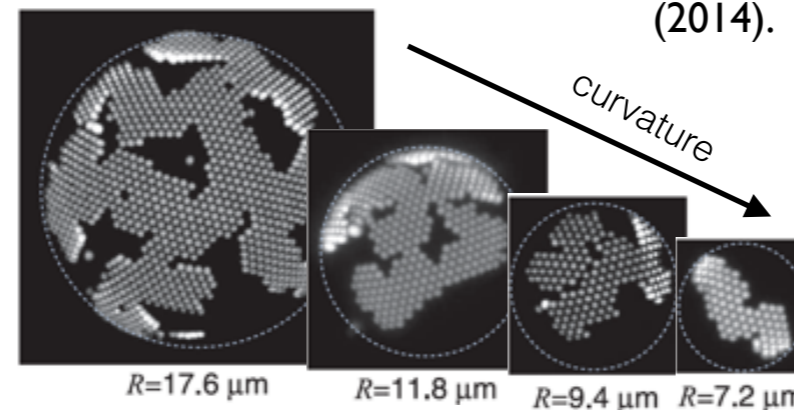
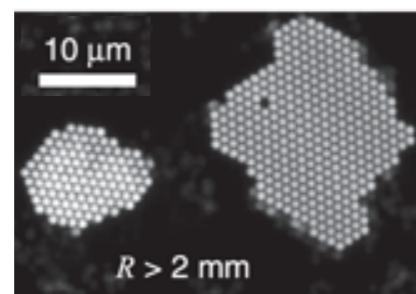
Bruss & GMG, *PNAS* (2012); *Soft Matter* (2013).

## IV) Perimeter Instability & Anisotropic Domains

### colloidal crystals on spherical droplets

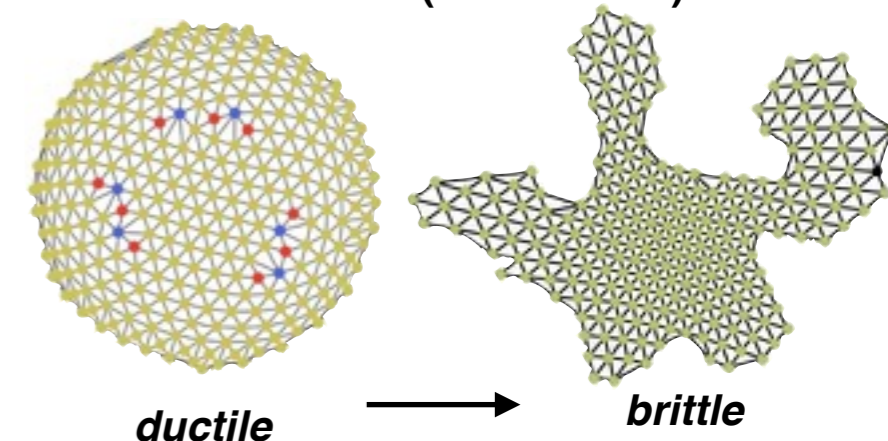


large droplets



Meng et al., *Science* (2014).

### cohesive membranes on spherical substrates (simulations)



Amir Azadi, to be published.



# Elastic Perimeter Instability of Curved Crystals

EUROPHYSICS LETTERS

1 April 2005

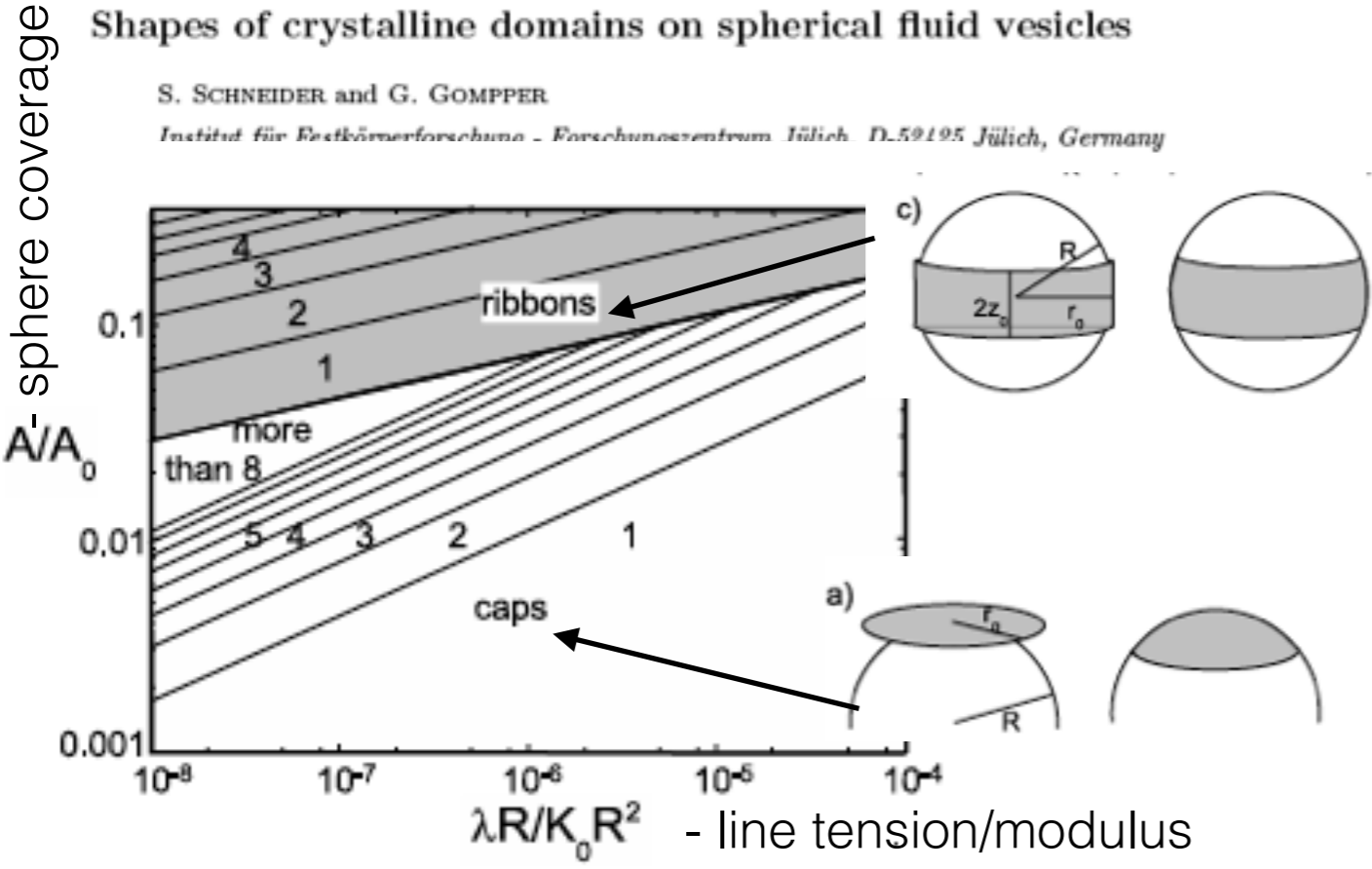
*Europhys. Lett.*, 70 (1), pp. 136–142 (2005)

DOI: 10.1209/epl/i2004-10464-2

## Shapes of crystalline domains on spherical fluid vesicles

S. SCHNEIDER and G. GOMPPER

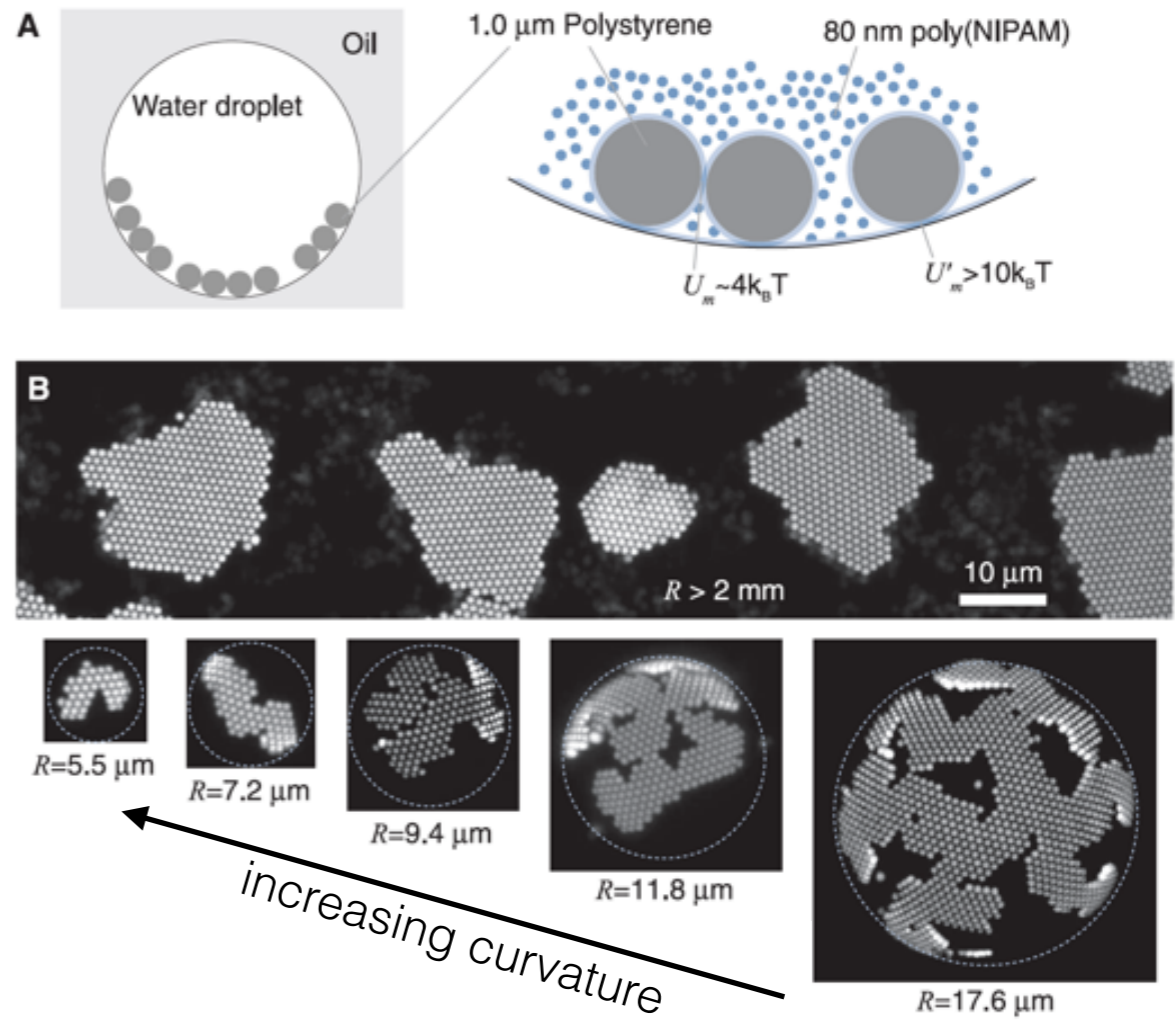
*Institut für Festkörperforschung - Forschungszentrum Jülich, D-52195 Jülich, Germany*



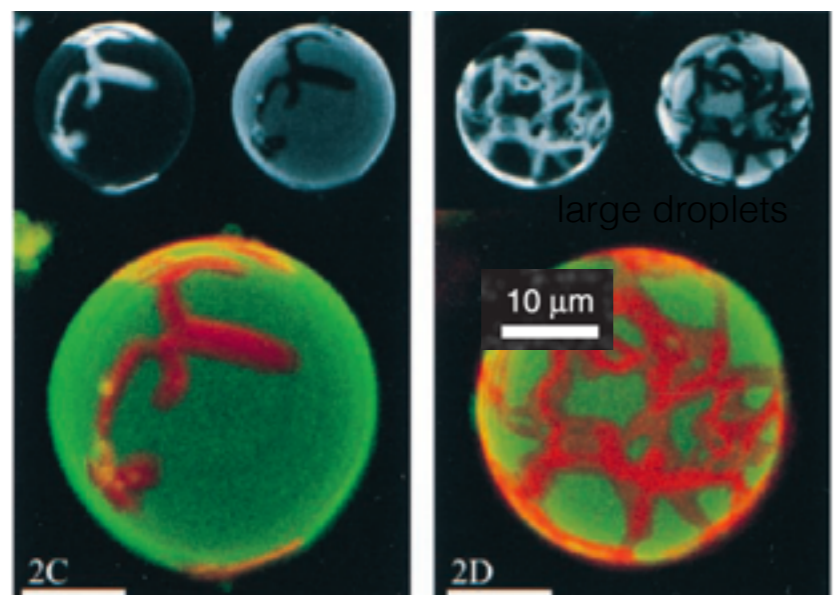
## Elastic Instability of a Crystal Growing on a Curved Surface

Guangnan Meng,<sup>1</sup> Jayson Paulose,<sup>2</sup> David R. Nelson,<sup>1,2</sup> Vinothan N. Manoharan<sup>2,1\*</sup>

7 FEBRUARY 2014 VOL 343 SCIENCE



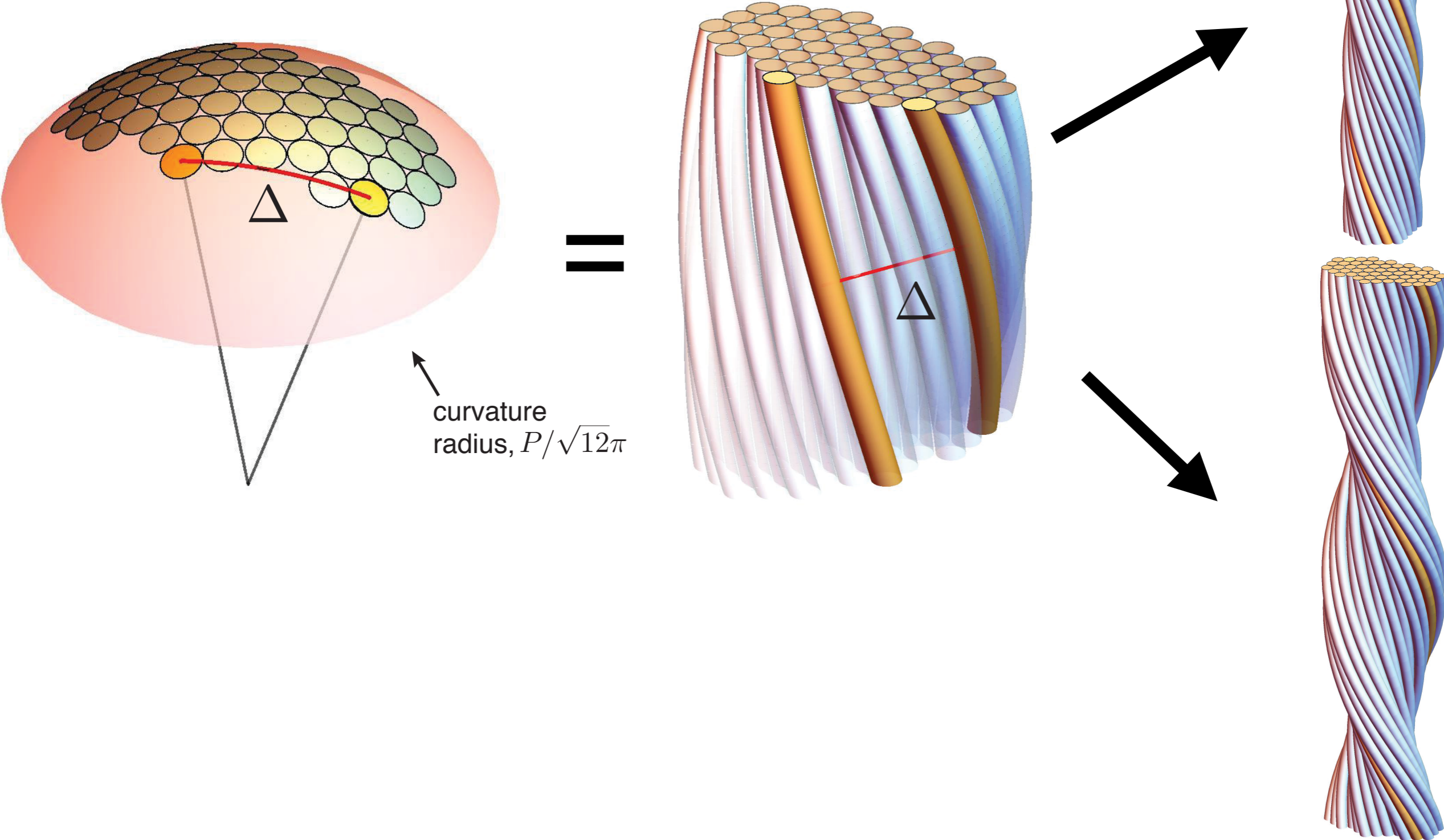
## lipid solid-fluid coexistence on GUVs



Webb *et al.* PNAS (1999).

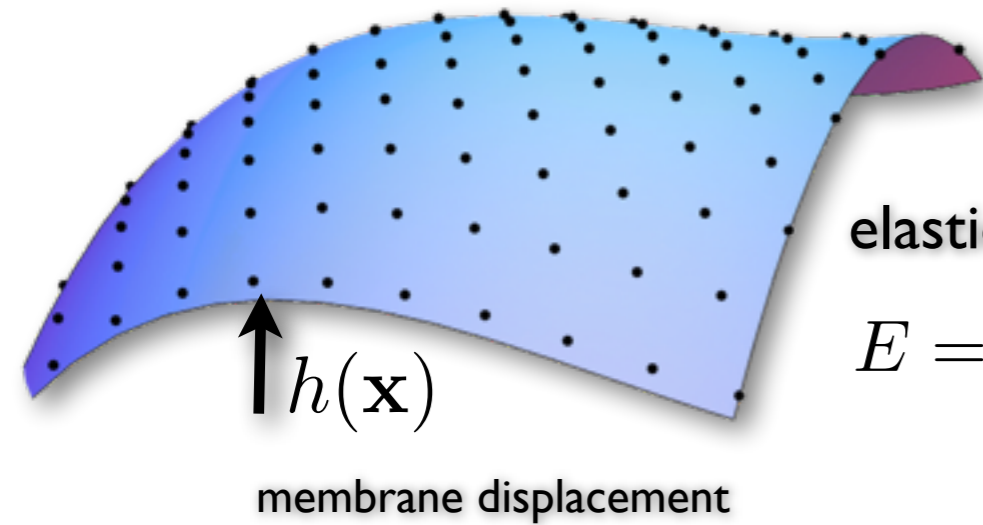


# How does metric frustration and boundary instability select optimal “morphology” of twisted bundles of chiral filaments?





# Curved Membranes vs. Twisted Bundles: Elasticity



in-plane stress:

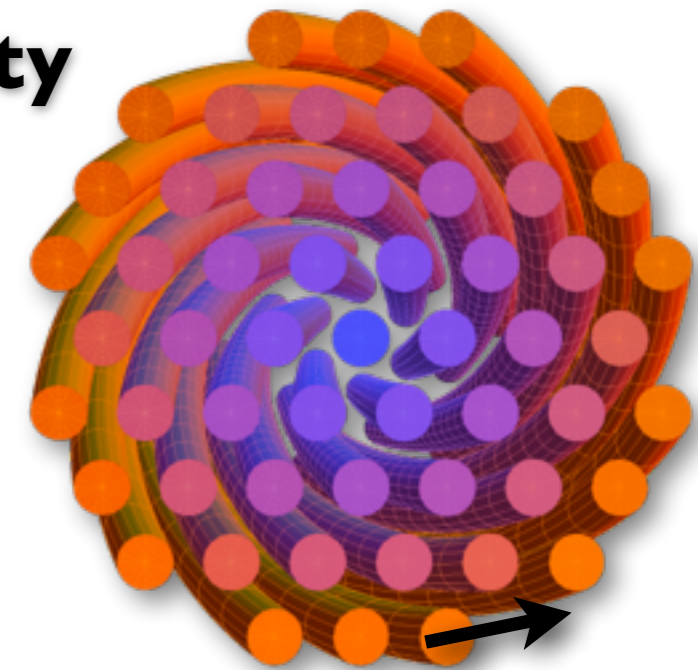
$$\sigma_{ij} = \lambda \delta_{ij} u_{kk} + 2\mu u_{ij}$$

elastic energy:

$$E = \frac{1}{2} \int dV \sigma_{ij} u_{ij}$$

Young's modulus:

$$Y = \frac{4\mu(\lambda + \mu)}{\lambda + 2\mu}$$



$$\mathbf{t}_\perp \simeq (\Omega\rho)\hat{\phi}$$

non-linear strain

$$u_{ij} = \frac{1}{2} (\partial_i u_j + \partial_j u_i + \partial_i h \partial_j h)$$

$$u_{ij}^\perp = \frac{1}{2} (\partial_i u_j + \partial_j u_i - t_i t_j)$$

Compatibility relation

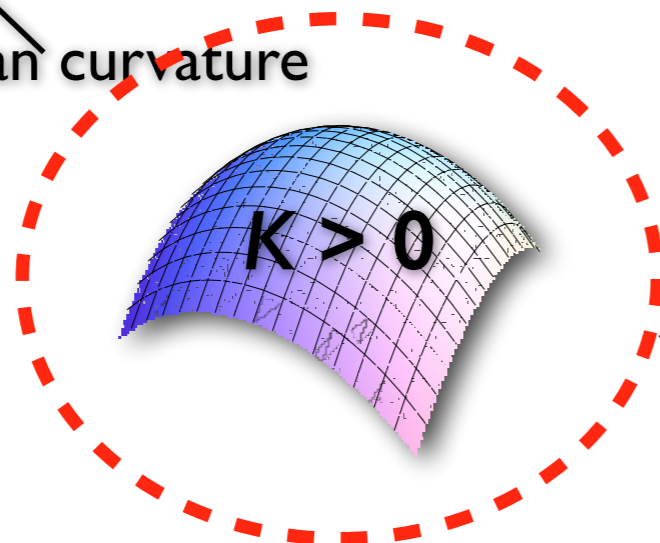
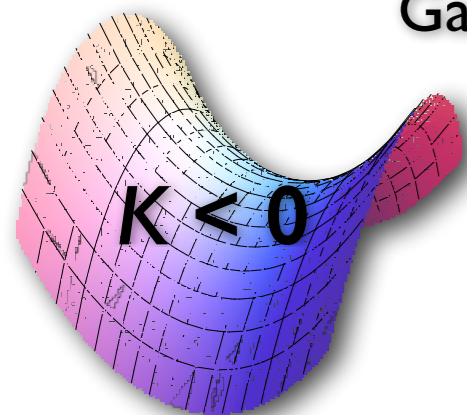
$$\frac{\nabla_\perp^2 \sigma_{ii}}{Y} = -(\partial_x^2 h)(\partial_y^2 h) + (\partial_x \partial_y h)^2$$

$$= -K$$

$$\frac{\nabla_\perp^2 \sigma_{ii}}{Y} = -\frac{1}{2} \left[ (\partial_x t_y)^2 + (\partial_y t_x)^2 - 2\partial_x \partial_y (t_x t_y) \right]$$

$$\equiv -K_{eff} = -3\Omega^2$$

Gaussian curvature



Bundle twist generates interfilament stress identical to **positive** Gaussian curvature in 2D membranes



# Isotropic, Twisted Cylindrical Bundles: Thermodynamics

*intra-filament*  
(bending) elasticity

*inter-filament*  
(packing) elasticity

surface energy  
(cohesion)

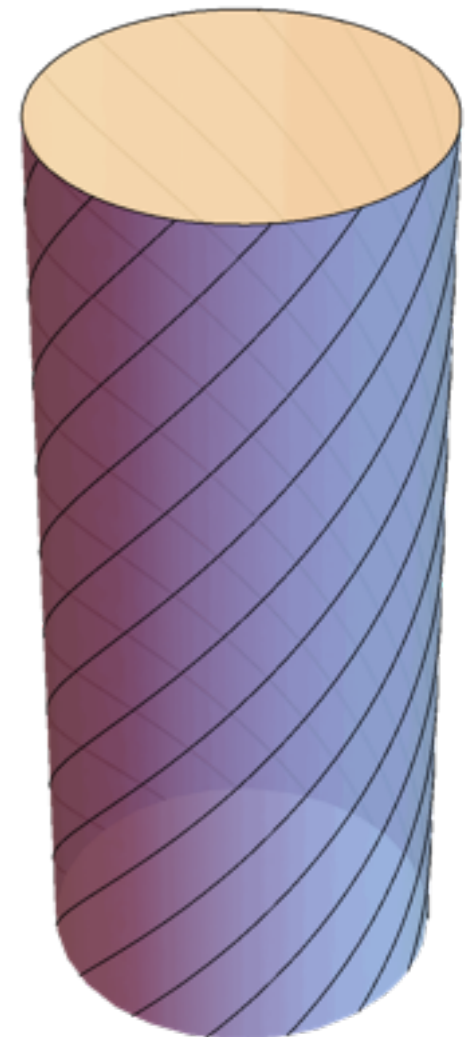
$R$  - bundle radius

$\Omega$  - twist ( $2\pi/\text{pitch}$ )

$$F = \frac{B\rho_0}{2} \int dV \kappa^2(r) + \frac{1}{2} \int dV \sigma_{ij} u_{ij} + \Sigma(2\pi RL)$$

$\kappa(r) \simeq \Omega^2 r$   
filament curv.

$\sigma_{ii} \approx -Y(\Omega R)^2$   
geometric strain





# Isotropic, Twisted Cylindrical Bundles: Thermodynamics

*intra-filament*  
(bending) elasticity

*inter-filament*  
(packing) elasticity

surface energy  
(cohesion)

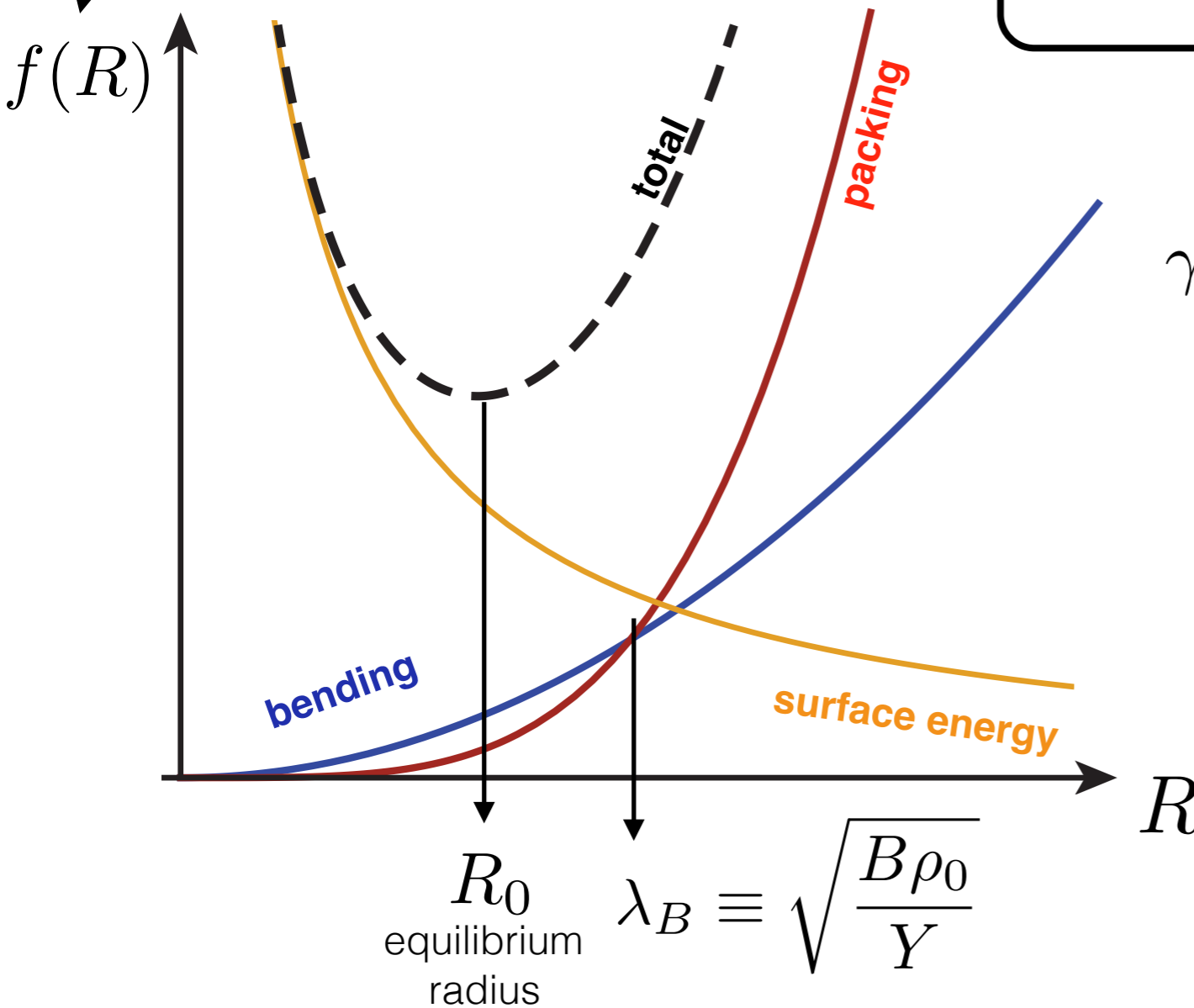
$R$  - bundle radius

$\Omega$  - twist ( $2\pi/\text{pitch}$ )

$$f(R) = \frac{B\rho_0}{4}\Omega^4 R^2 + \frac{3Y}{128}(\Omega R)^4 + \frac{2\Sigma}{R}$$

free-energy density

$$\gamma \equiv (R_0/\lambda_B)^2 = \frac{\text{"packing" cost}}{\text{bending cost}}$$

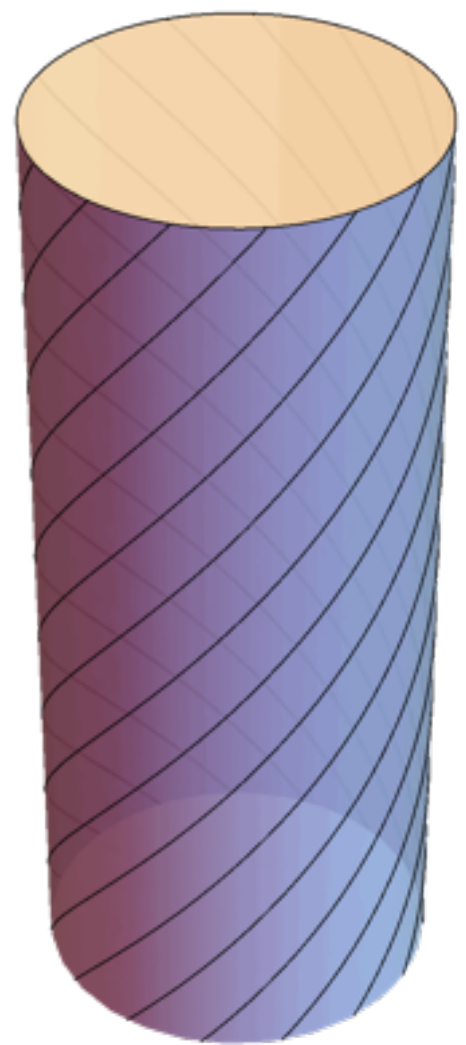


$\gamma \ll 1$ : **bending** limited

$$R_0 \sim (\Sigma/B\Omega^4)^{1/3}$$

$\gamma \gg 1$ : **packing** limited

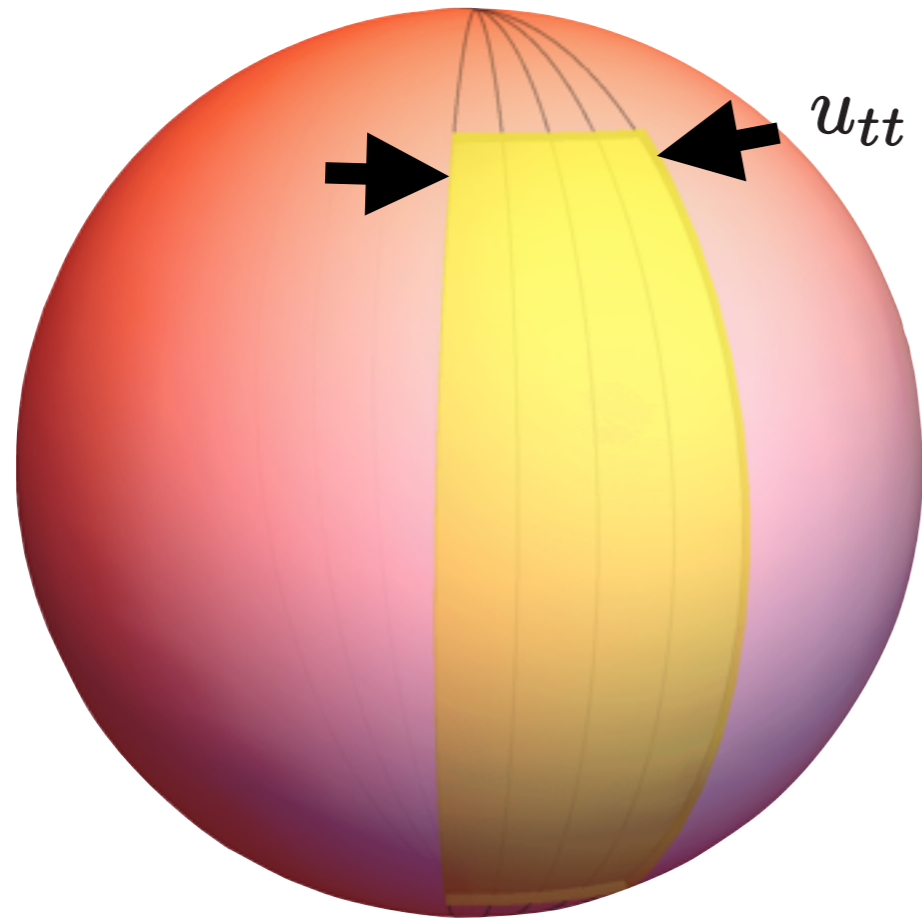
$$R_0 \sim (\Sigma/Y\Omega^4)^{1/5}$$





# Anisotropic, Helical "Tapes": Inter- vs. Intra-filament Strain

width preserving map

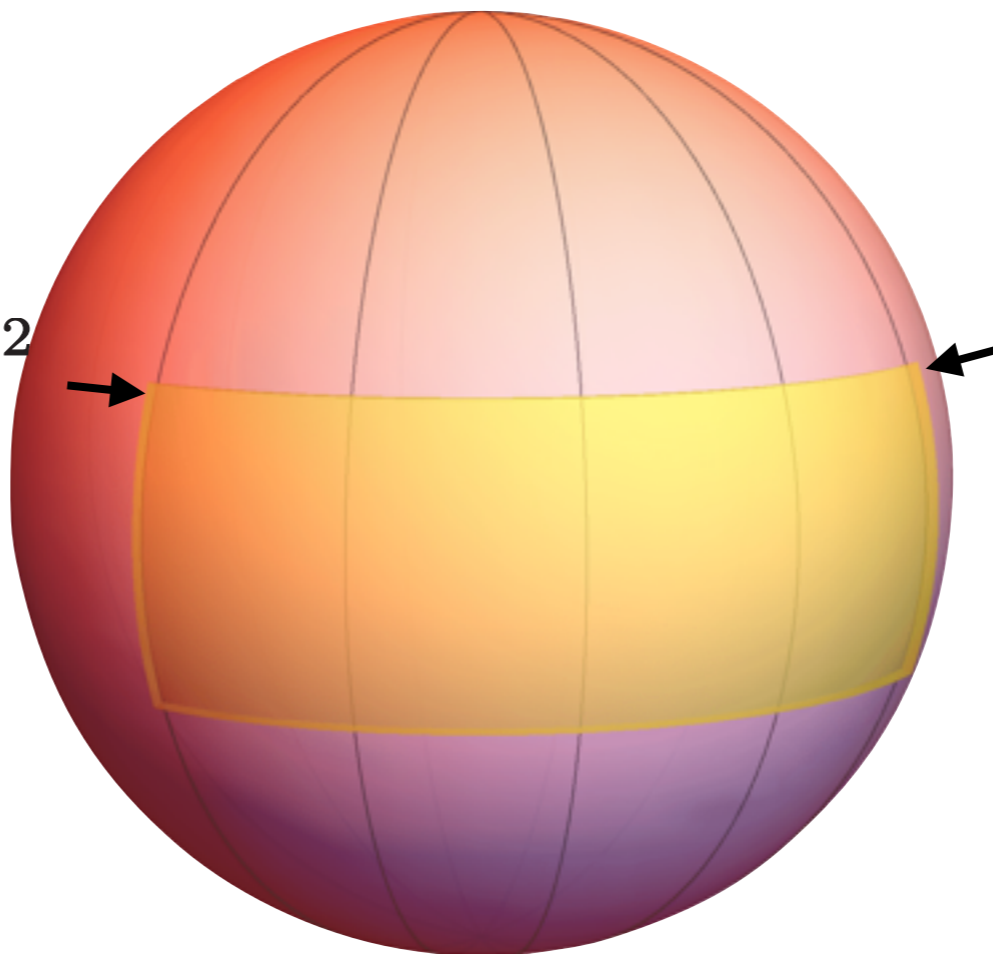


$$u_{tt} \approx -\left(\frac{w}{R_s}\right)^2$$

strain grows with  
wide dimension

⇒ **large elastic energy**

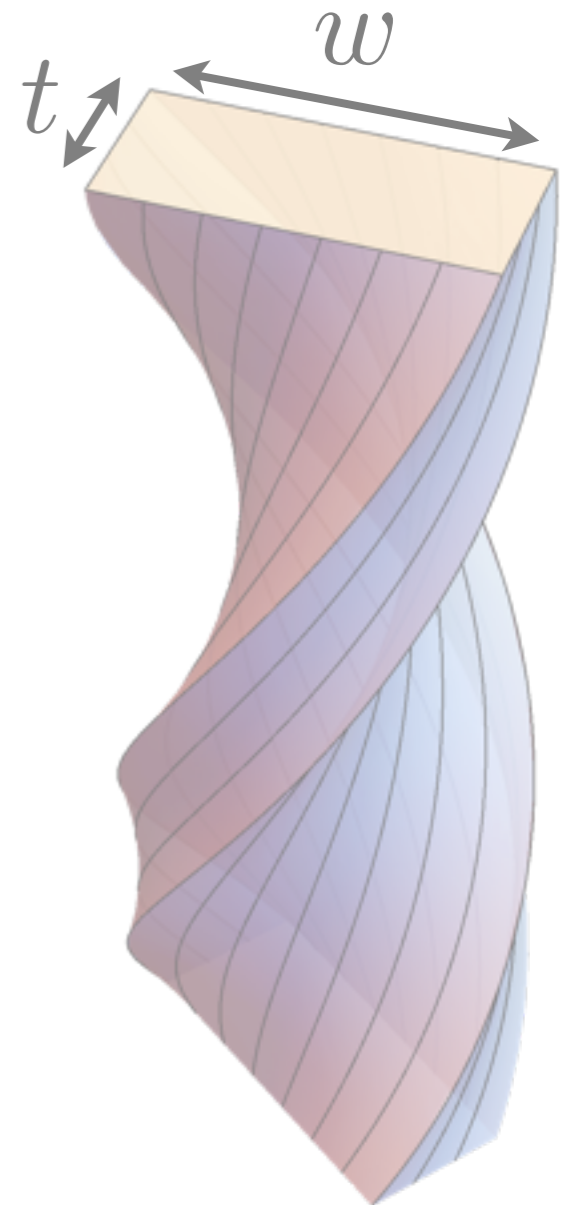
thickness preserving map



$$u_{ww} \approx -\left(\frac{t}{R_s}\right)^2$$

strain grows with  
*thin* dimension

⇓  
**low elastic energy**





# Anisotropic, Helical “Tapes”: Inter- vs. Intra-filament Strain

*intra-filament*  
(bending) elasticity

*inter-filament*  
(packing) elasticity

surface energy  
(cohesion)

$$f(w \gg t) \simeq \frac{B\rho_0}{24} \Omega^4 w^2 + \frac{Y}{160} (\Omega t)^4 + 2\Sigma \left( \frac{1}{w} + \frac{1}{t} \right)$$

$\swarrow$   $\kappa \approx \Omega^2 w$        $\swarrow$   $u_{ww} \approx -(t/R_s)^2$

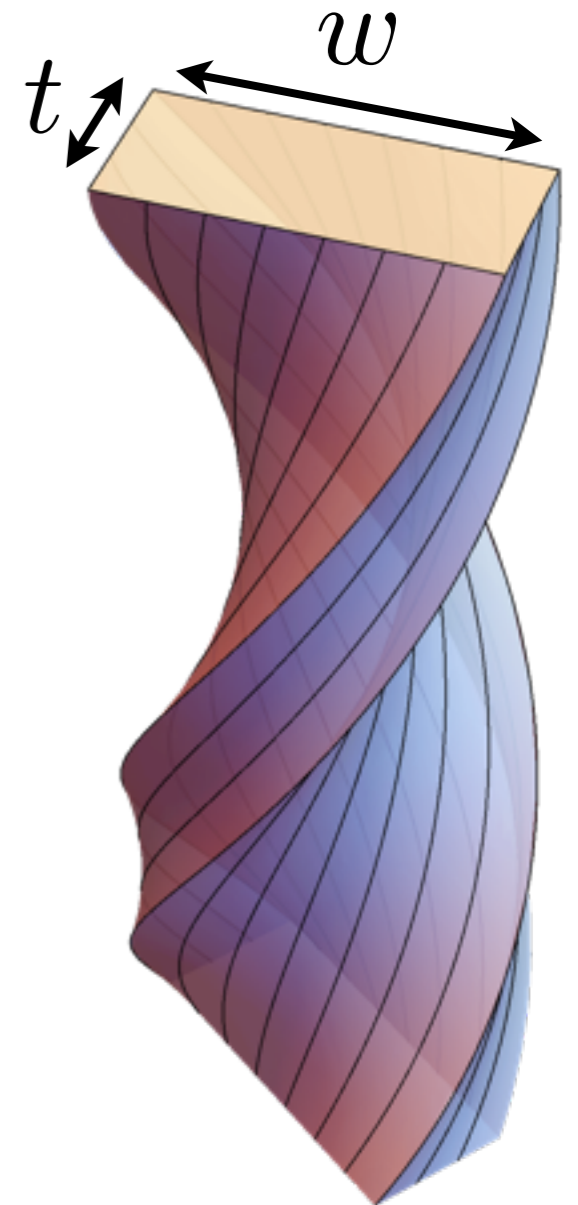
equilibrium dimensions

tape width: **bending** limited

$$w_0 = 24^{1/3} \left( \frac{\Sigma}{\Omega^4 B\rho_0} \right)^{1/3}$$

tape thickness: **packing** limited

$$t_0 = 80^{1/5} \left( \frac{\Sigma}{\Omega^4 Y} \right)^{1/5}$$



# From Bundles to Tapes: Critical Bundle Size

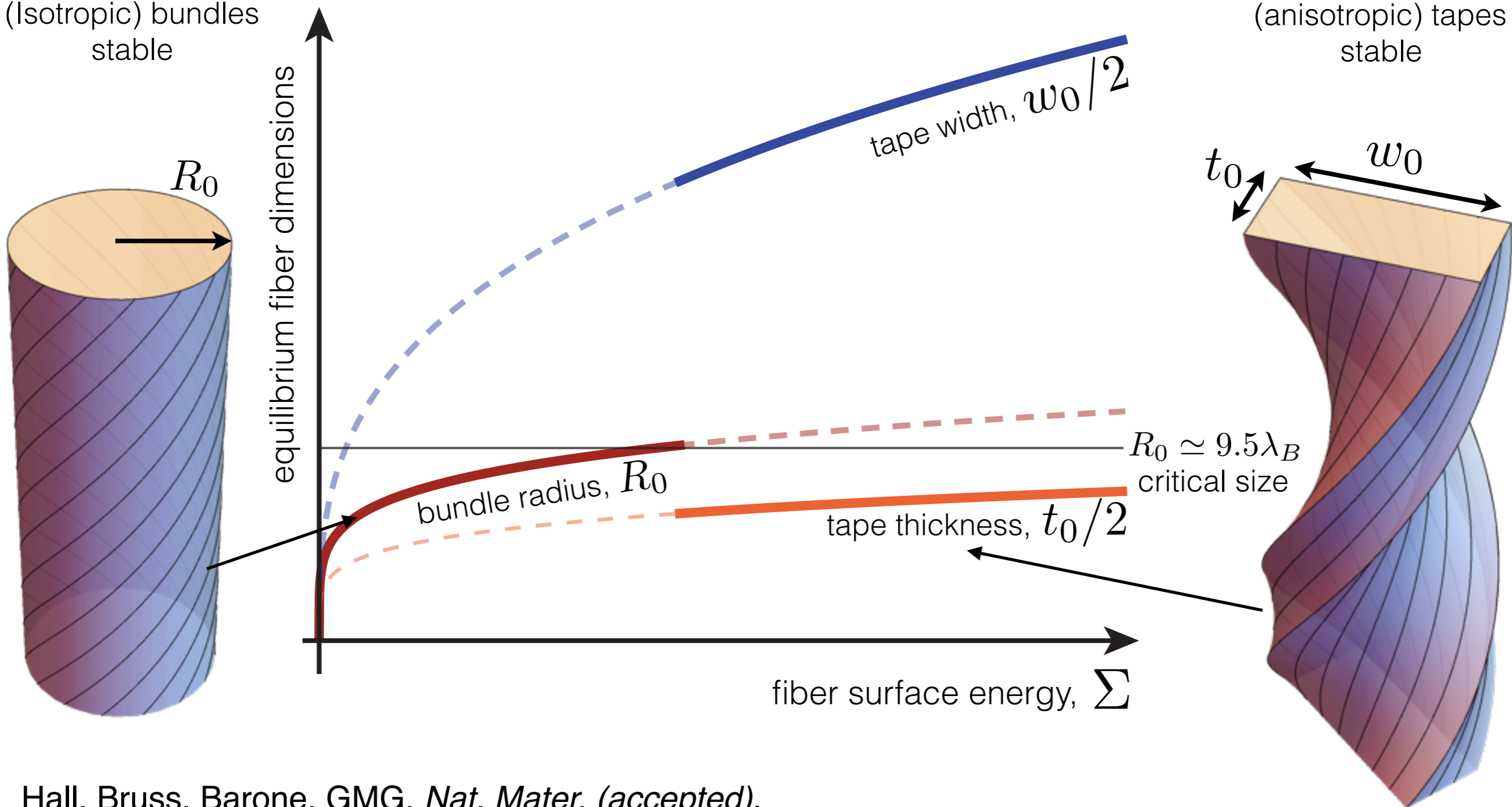
$$\gamma \equiv (R_0/\lambda_B)^2 = \frac{\text{"packing" cost}}{\text{bending cost}}$$

$$\gamma < 90.3$$

(Isotropic) bundles stable

$$\gamma > 90.3$$

(anisotropic) tapes stable



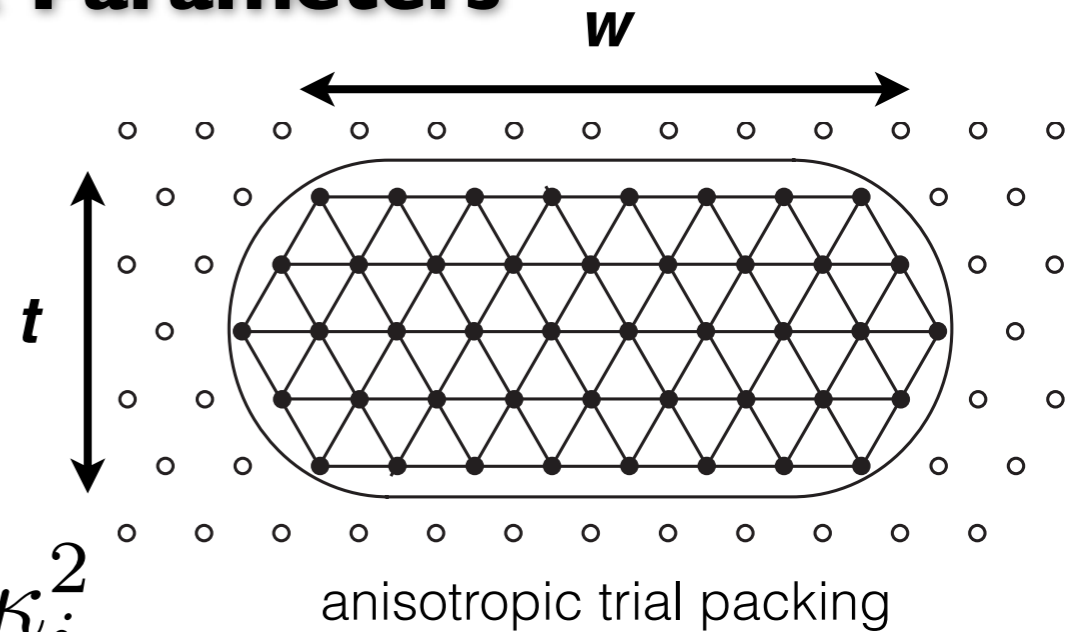


# Discrete filament simulations: Model & Parameters



Doug Hall (UMass)

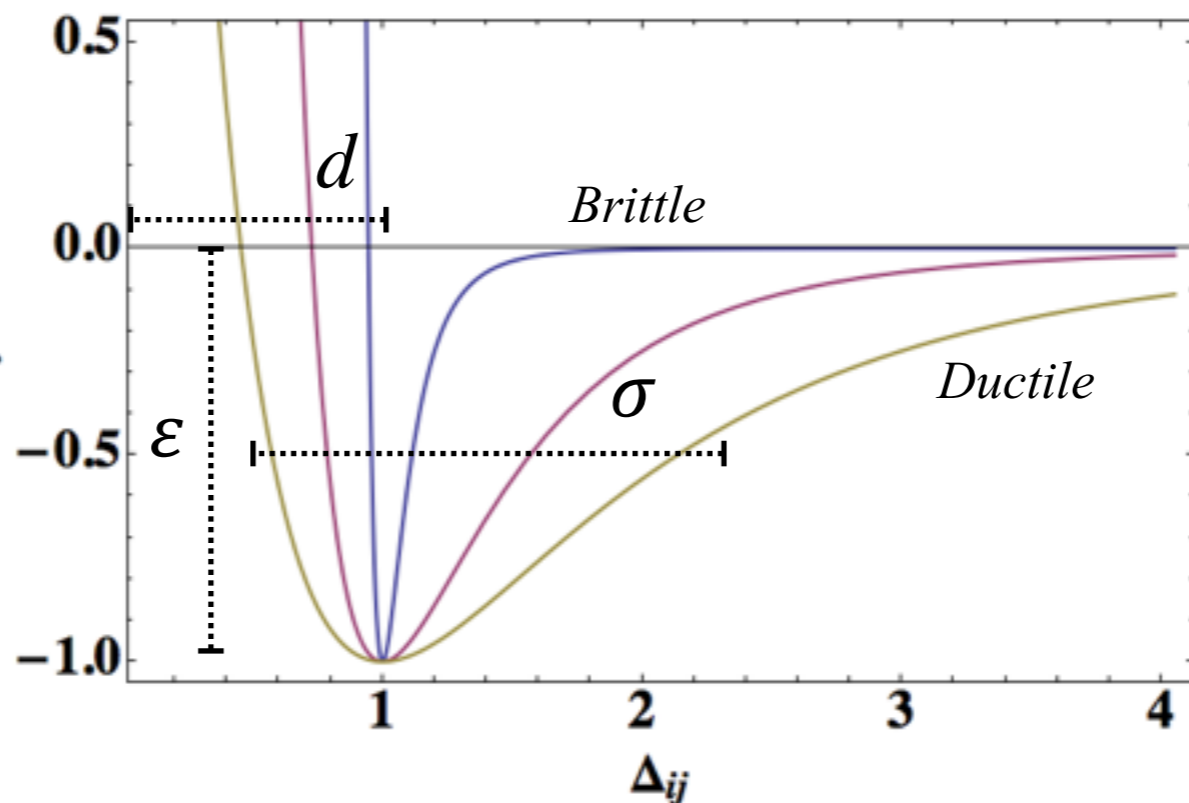
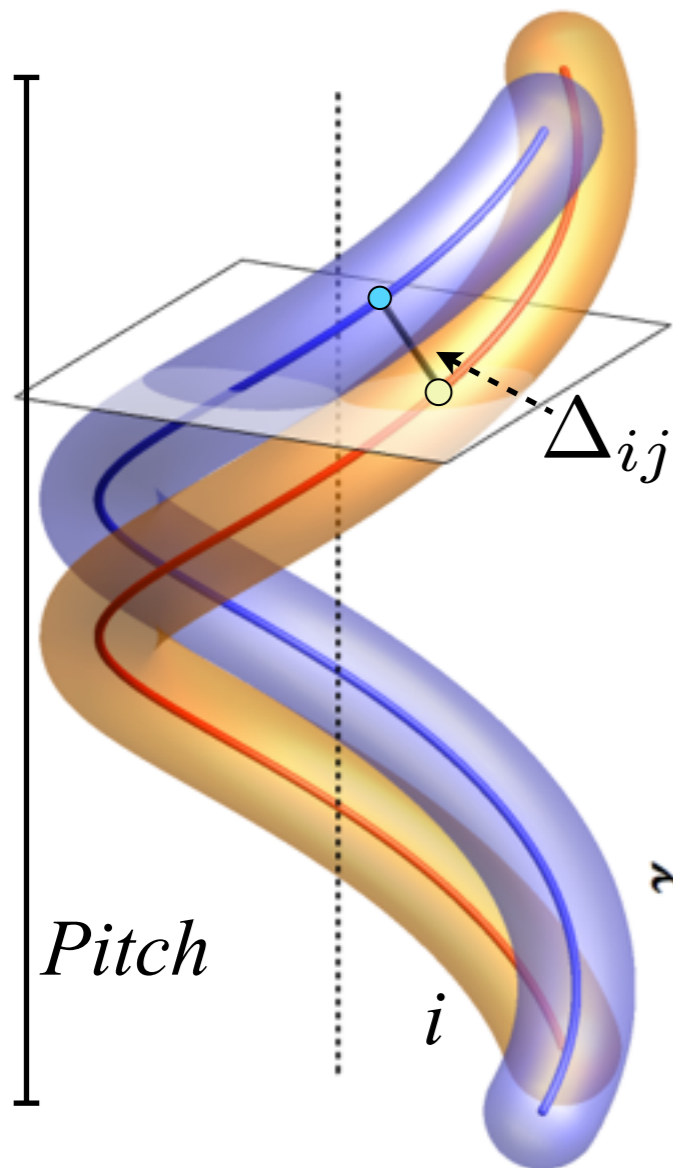
**Method:** (numerically) optimize 2D cross-section and  $N$  of filament bundles of fixed twist interacting via attractive, pair-wise forces



$$E_{Bend} = \frac{B}{2} L \sum_i \kappa_i^2$$

*Curvature*

$$E_{co} = \sum_{ij} \underbrace{L_{ij}}_{\text{Length}} \underbrace{\gamma(\Delta_{ij})}_{\text{Energy per unit length}}$$



$$\lambda_B \equiv \sqrt{\frac{B\rho_0}{Y}}$$

$$\propto (B/\epsilon)^{1/2} (d/\sigma)$$

$$\lambda_S \equiv \Sigma/Y$$

$$\propto d(\sigma/d)^2$$



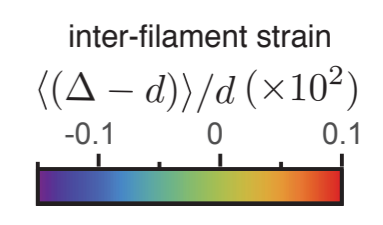
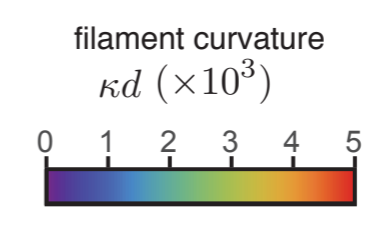
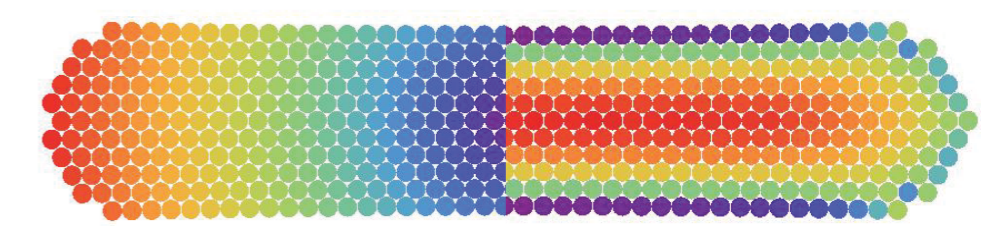
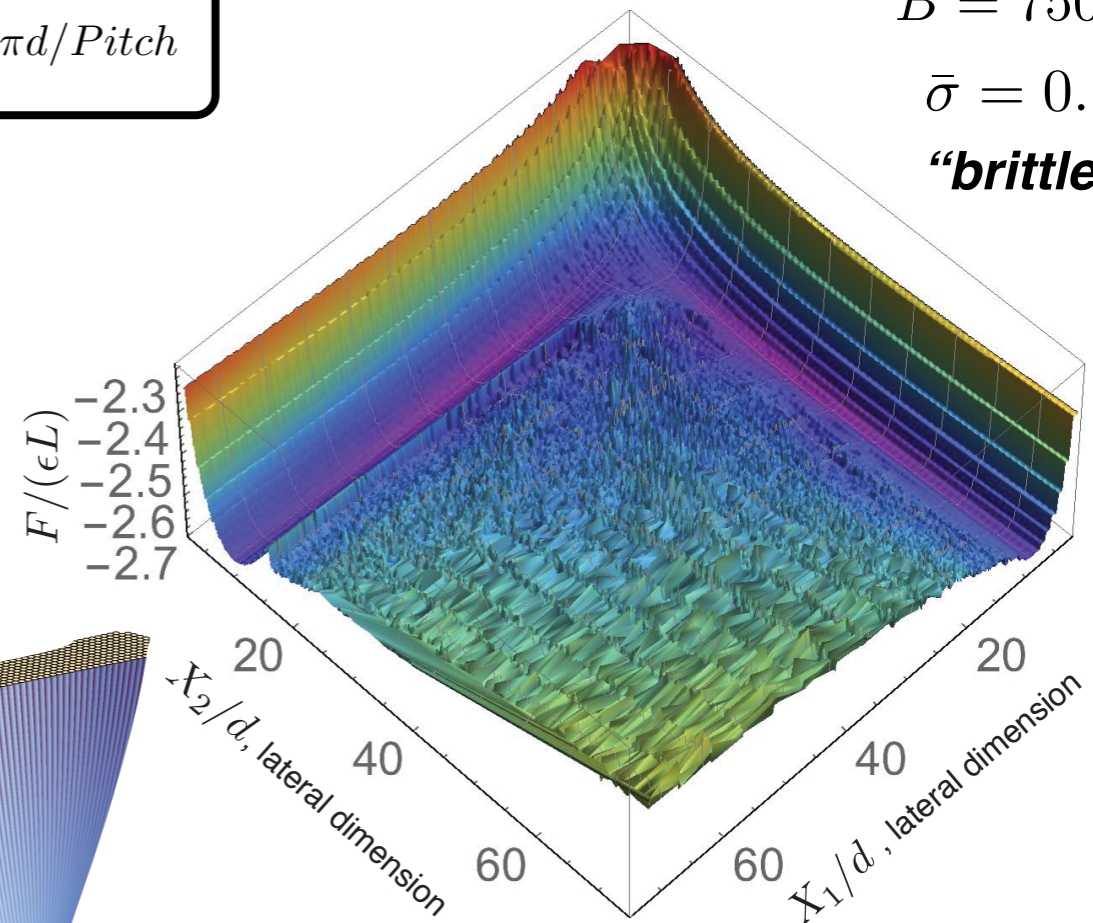
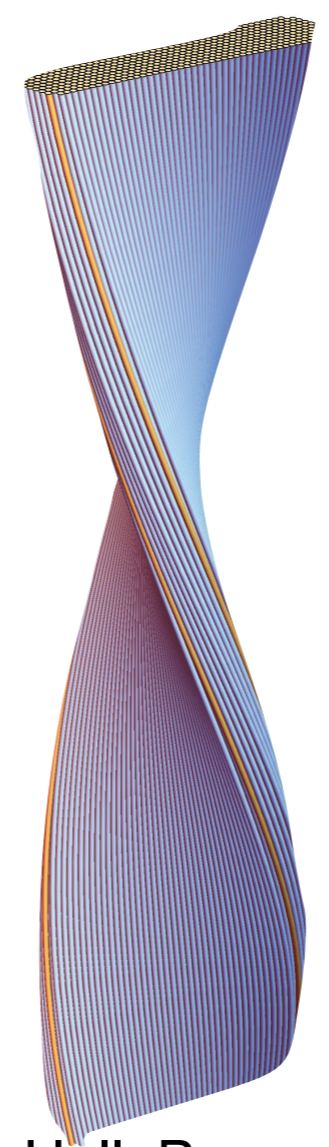
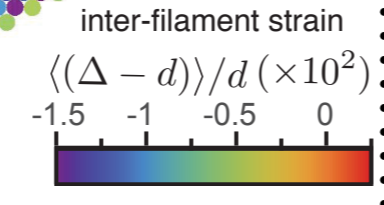
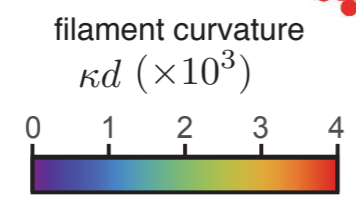
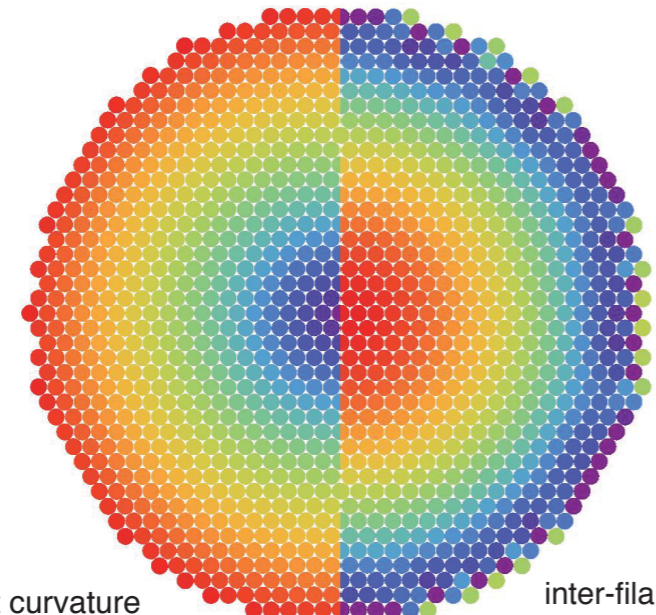
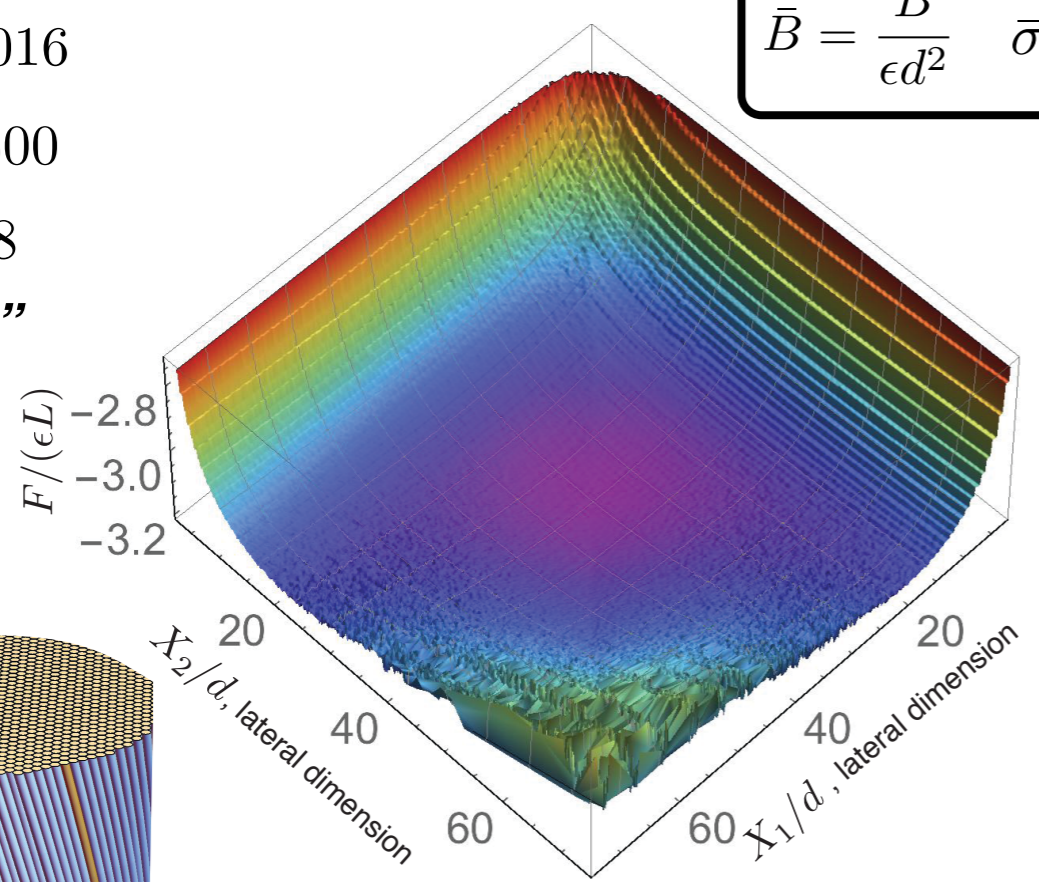
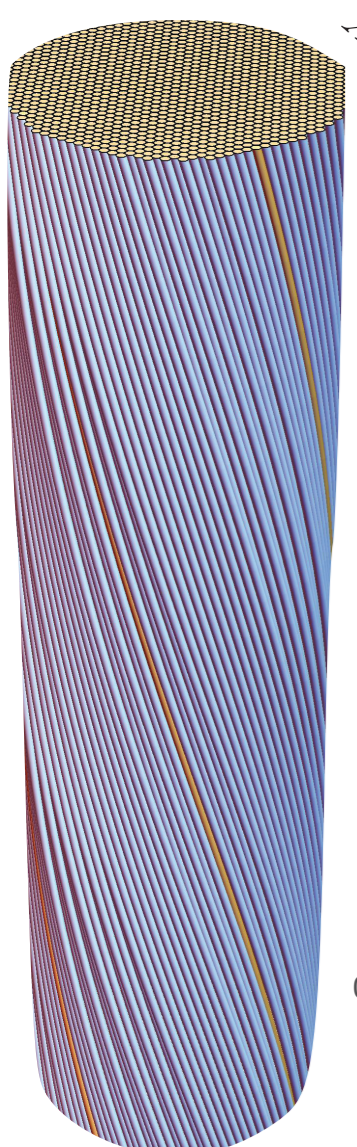
# Discrete filament simulations: Energy Landscapes & Optimal Morphologies

**scaled parameters:**

$$\bar{B} = \frac{B}{\epsilon d^2} \quad \bar{\sigma} = \frac{\sigma}{d} \quad \bar{\Omega} = 2\pi d / \text{Pitch}$$

$\bar{\Omega} = 0.016$   
 $\bar{B} = 7500$   
 $\bar{\sigma} = 0.8$   
**“ductile”**

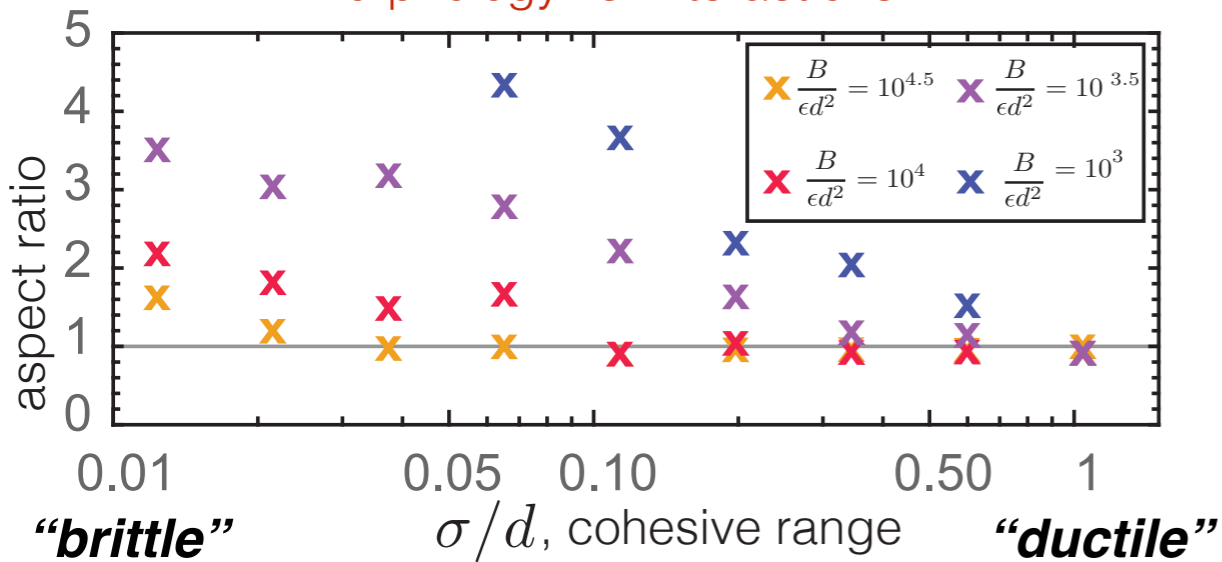
$\bar{\Omega} = 0.016$   
 $\bar{B} = 7500$   
 $\bar{\sigma} = 0.1$   
**“brittle”**





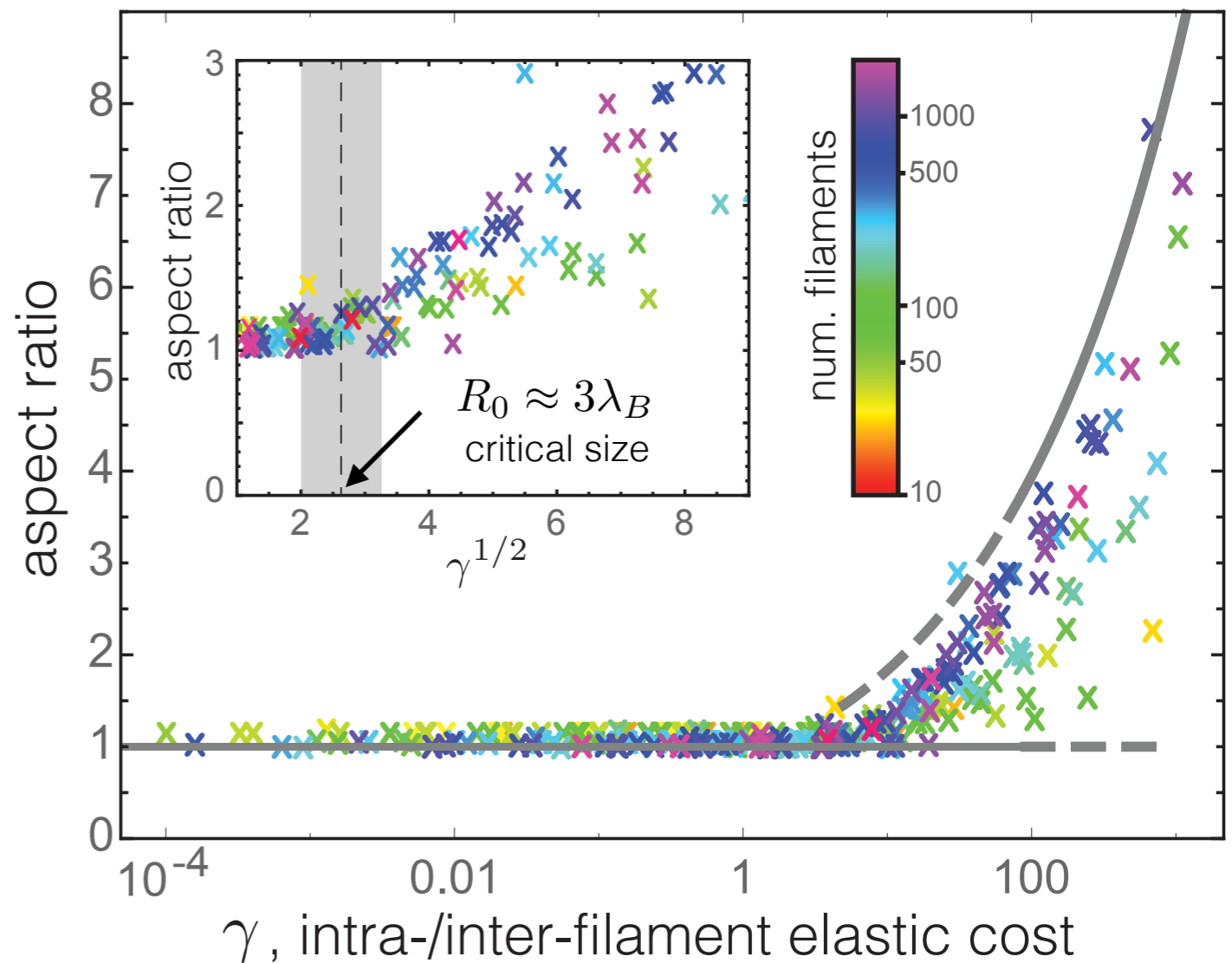
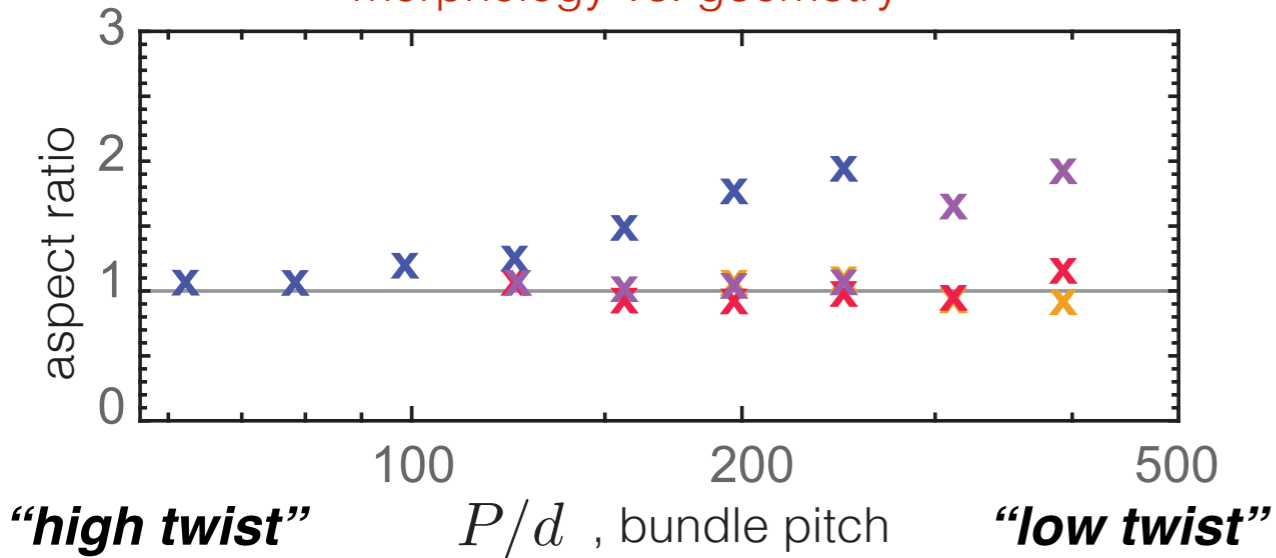
# Discrete filament simulations: Equilibrium aspect ratio

morphology vs. interactions



$$\gamma \equiv \left( R_0 / \lambda_B \right)^2 = \frac{\text{“packing” cost}}{\text{bending cost}}$$

morphology vs. geometry



# Twisted Amyloid Tapes: From Mesoscale Dimensions to “Molecular” Scale Parameters

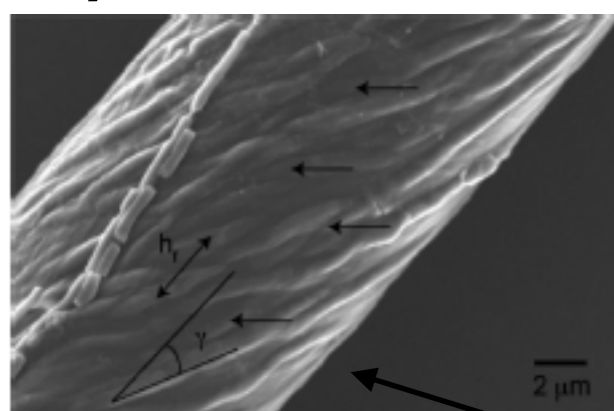
## Evolution of the Amyloid Fiber over Multiple Length Scales

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www.acsnano.org

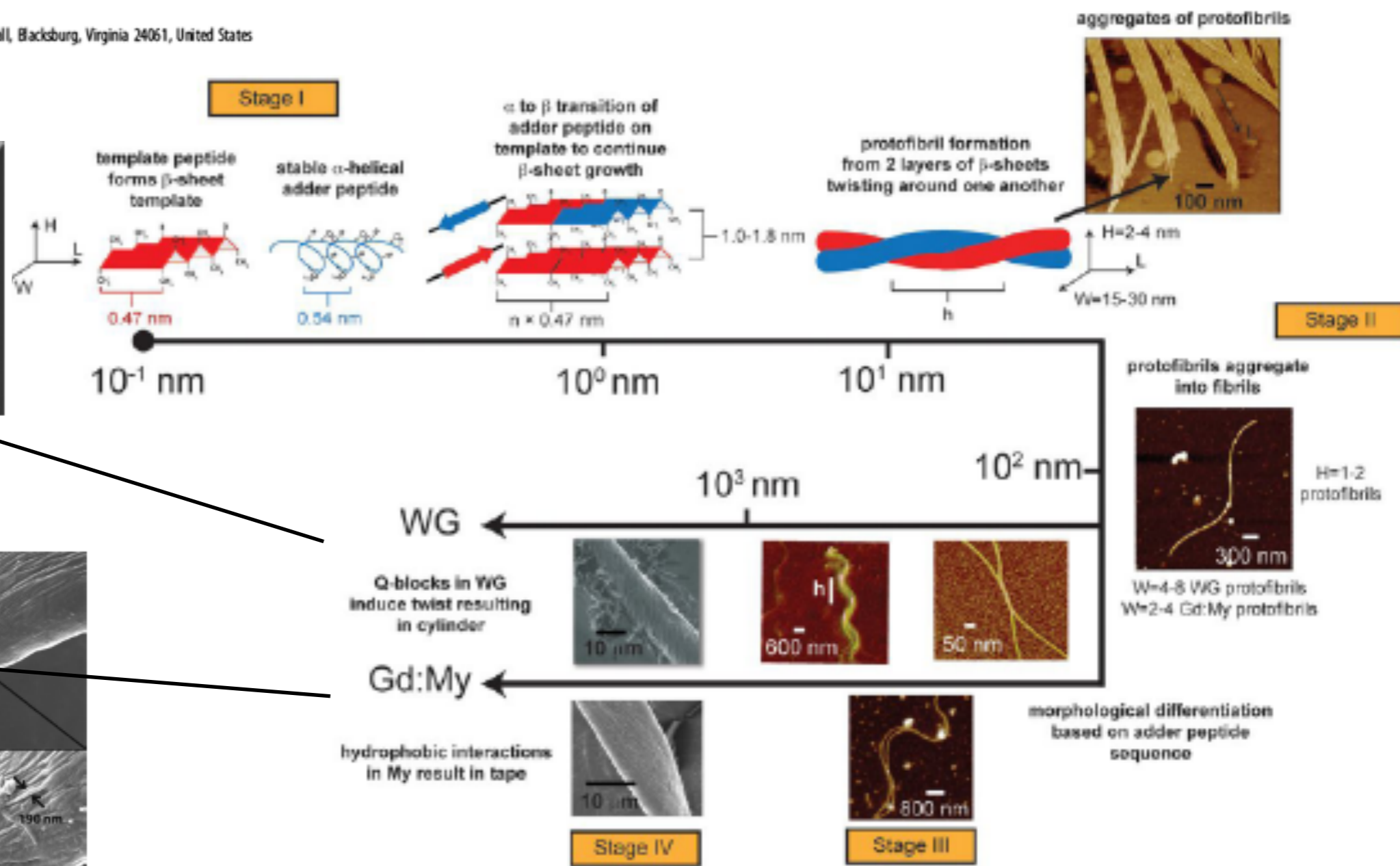
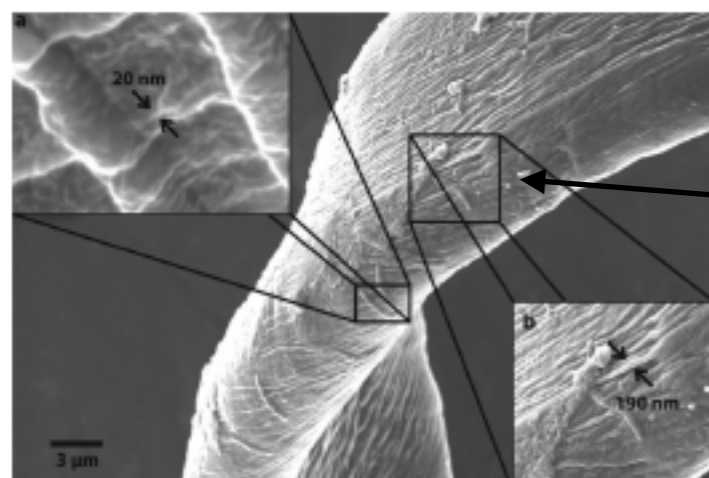
Devin M. Ridgley and Justin R. Barone\*

Biological Systems Engineering Department, Virginia Tech, 303 Seitz Hall, Blacksburg, Virginia 24061, United States

cylindrical fiber



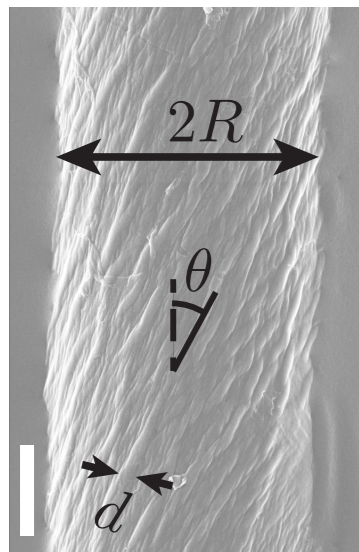
helical tape



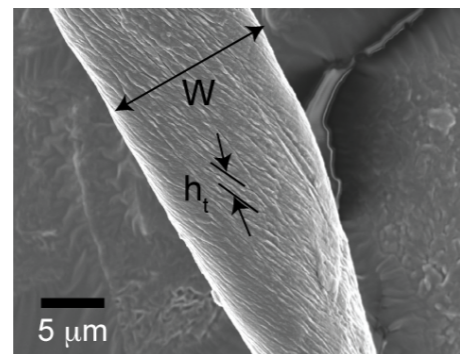
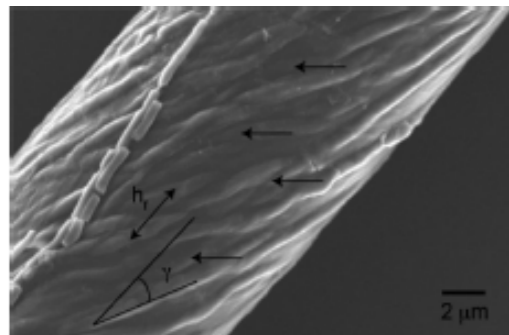
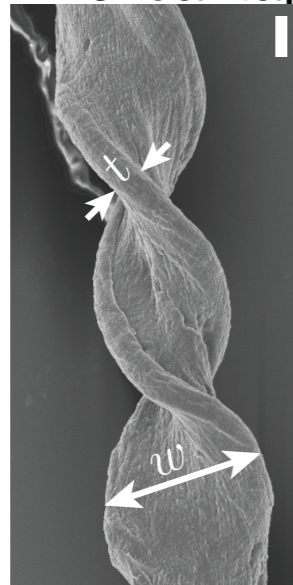


# Twisted Amyloid Tapes: From Mesoscale Dimensions to “Molecular” Scale Parameters

cylindrical bundles

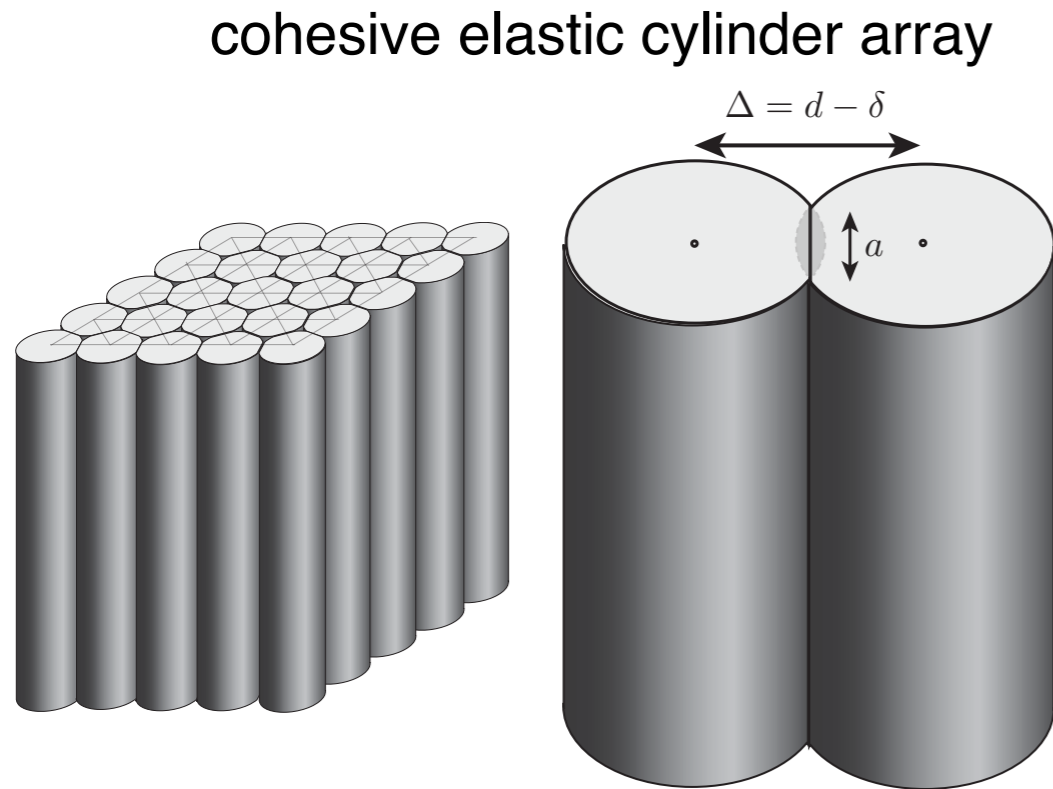


helical tapes



		pH				100 mM NaCl
$T$		4	6	8	10	
22 °C	WG			—		
	Gd:My			●/—		
37 °C	WG	●	●/—	●	●/—	—
	Gd:My	●/—	—	●/—	—	—
60 °C	WG			—		
	Gd:My			●/—		
80 °C	WG			—		
	Gd:My			●/—		

# Twisted Amyloid Tapes: From Mesoscale Dimensions to “Molecular” Scale Parameters



predicted tape dimensions:

$$w_0 = 24^{1/3} \left( \frac{\Sigma}{\Omega^4 B \rho_0} \right)^{1/3} \quad t_0 = 80^{1/5} \left( \frac{\Sigma}{\Omega^4 Y} \right)^{1/5}$$

characteristic lengths (material dependent):

$$\lambda_B \equiv \sqrt{\frac{B \rho_0}{Y}} = \sqrt{\frac{3t_0^5}{10w_0^3}} \quad \lambda_S \equiv \Sigma/Y = \frac{\Omega^4 t_0^5}{80}$$

array modulus

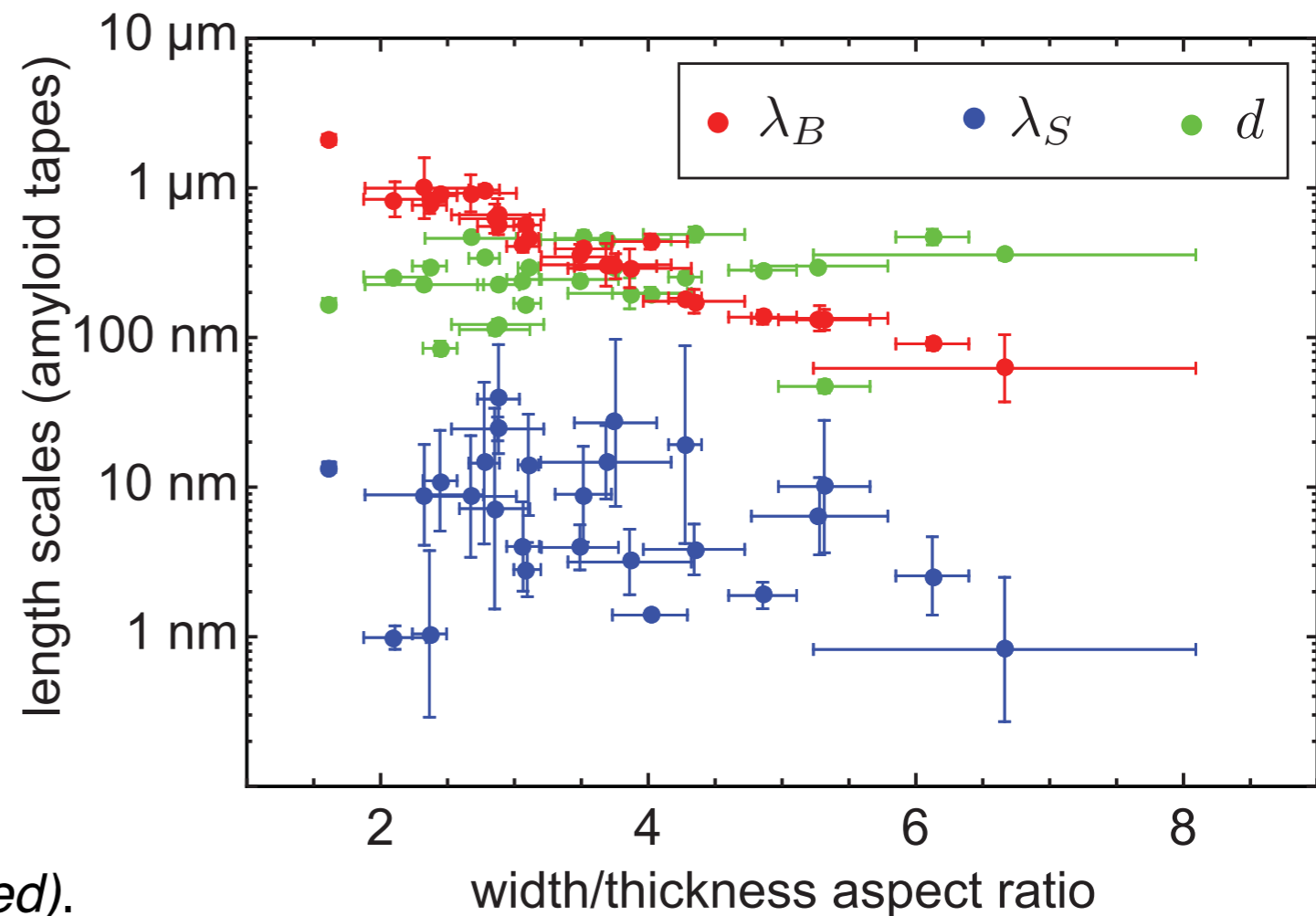
filament modulus

$$Y \approx E \Rightarrow \lambda_B \sim d$$

$$\rho_0 B \approx E d^2$$

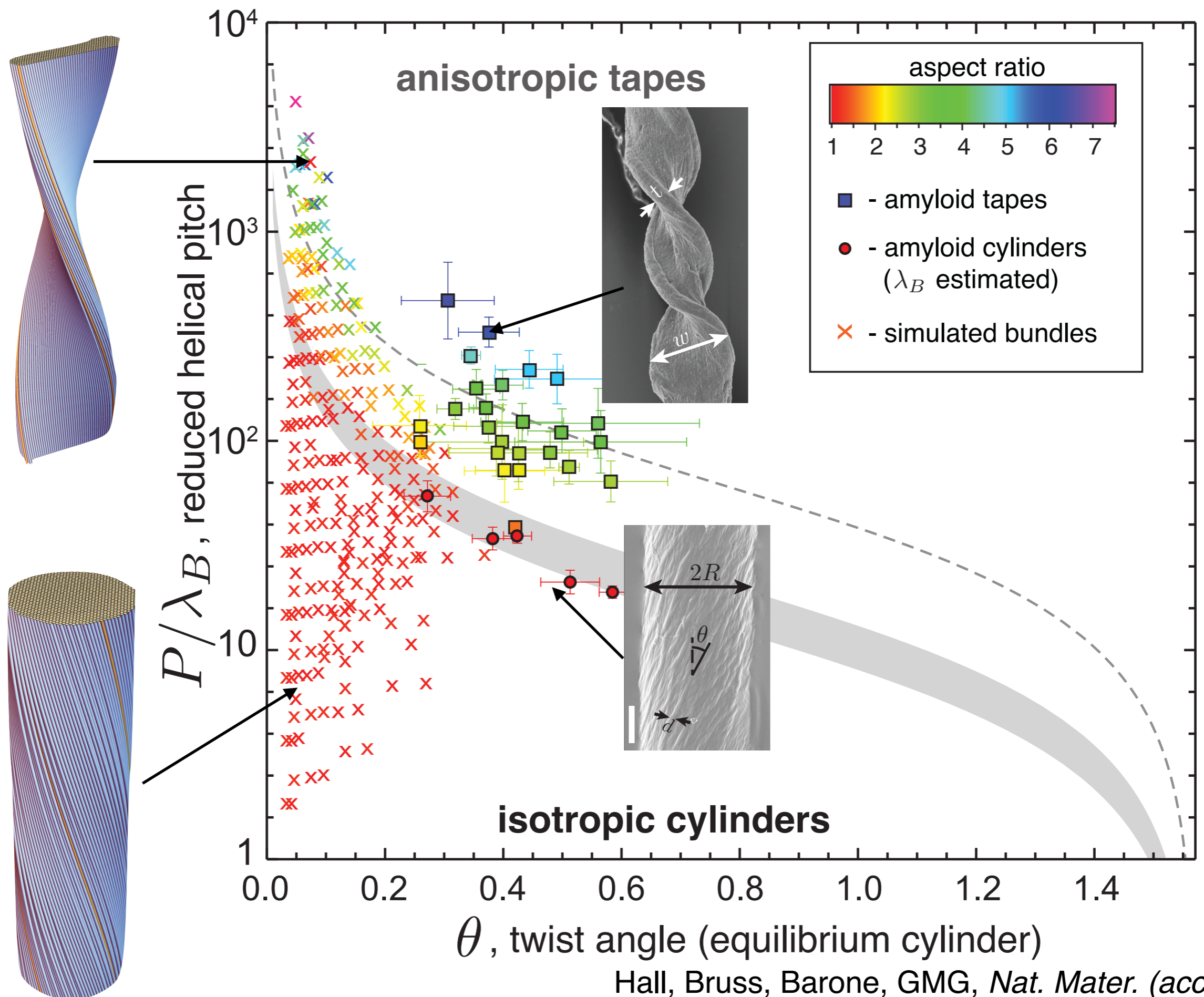
$$\sigma \sim \delta \Rightarrow \lambda_S \sim \delta^2 / d \ll d$$

cohesive range      contact “depth”





# Bundle morphology: a universal phase diagram



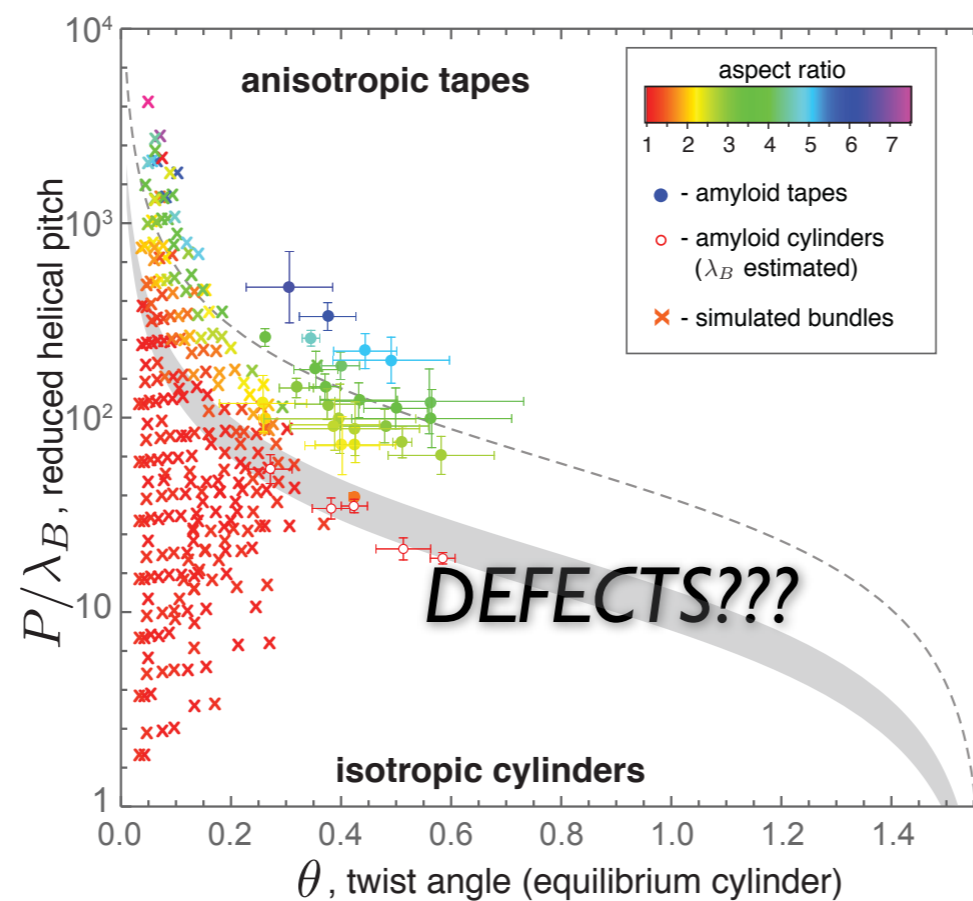
# Summary (Frustration & Morphology Selection):

- 1) Geometric strains drive anisotropy in fiber sections above critical size
- 2) Tape **width/thickness** dimensions are selected by **intra-filament (bending)/intra-filament (packing) elasticity**
- 3) Mesoscale dimensions directly quantify microscopic parameters (**inter-filament elasticity; intra-filament elasticity; inter-fil. cohesion**)

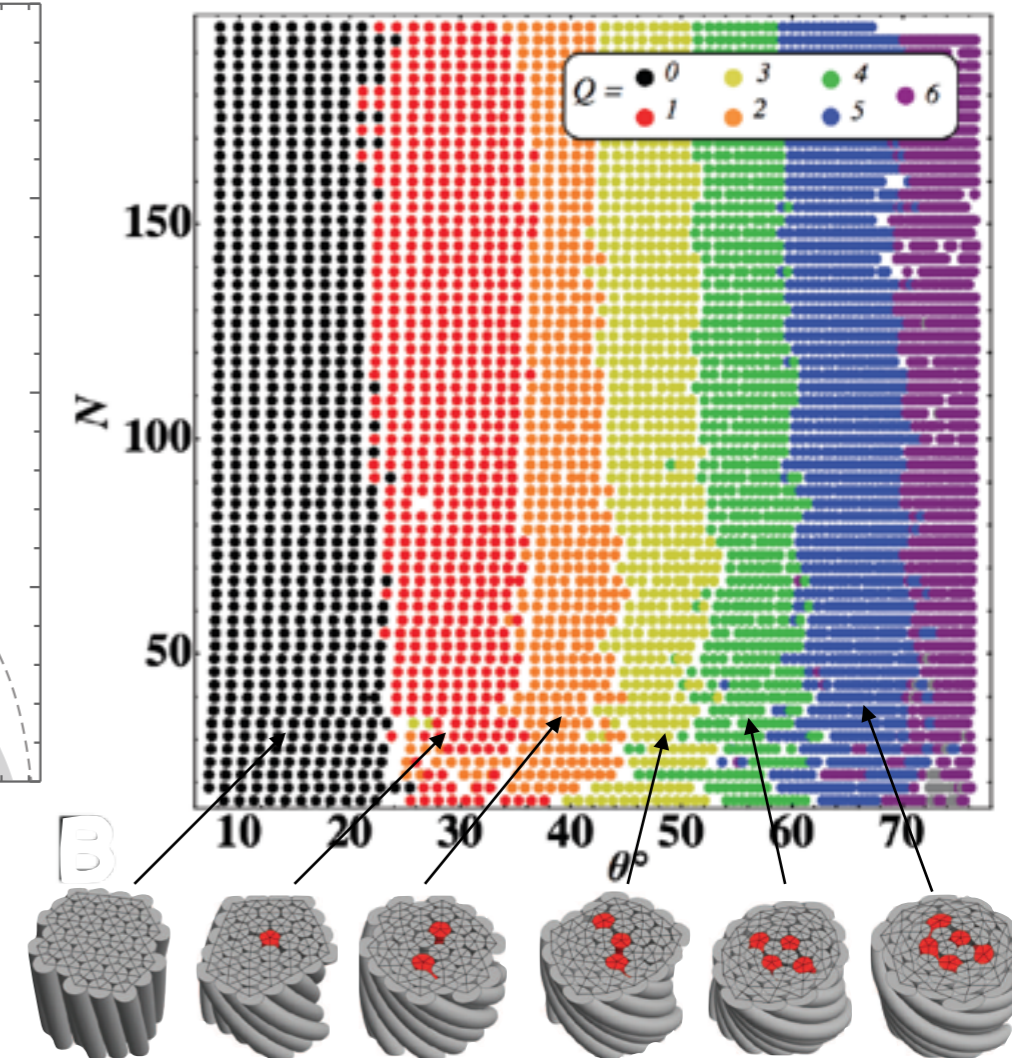
## Open questions:

Stiff filaments at large twist?

How do defects mitigate bundle/tape transition & alter self-limitation?



Disclinations in twisted bundles  
(Bruss & GMG PNAS, 2012; Soft Matter 2013)

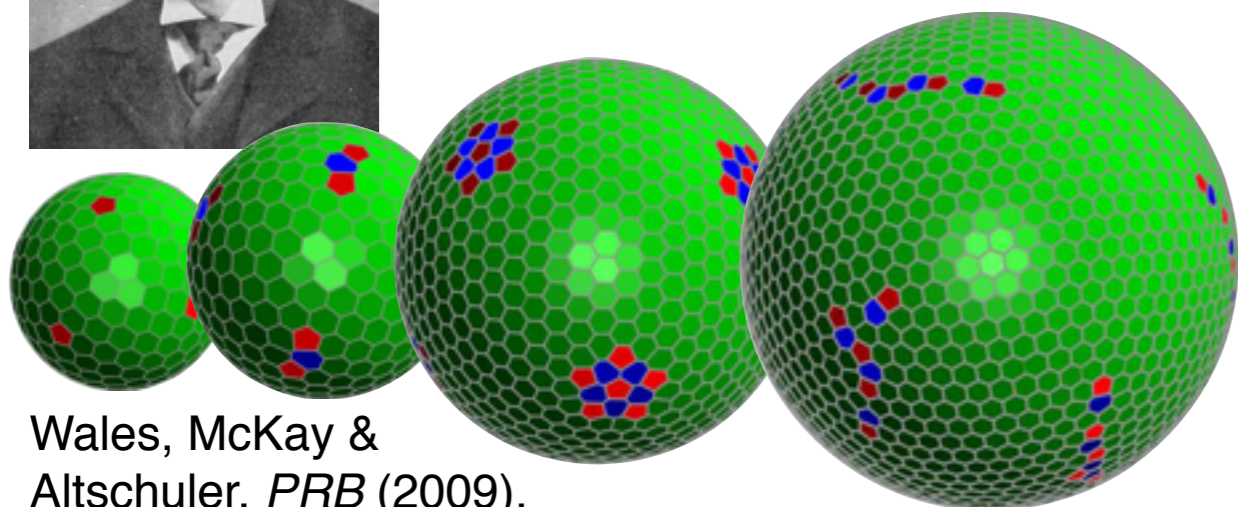




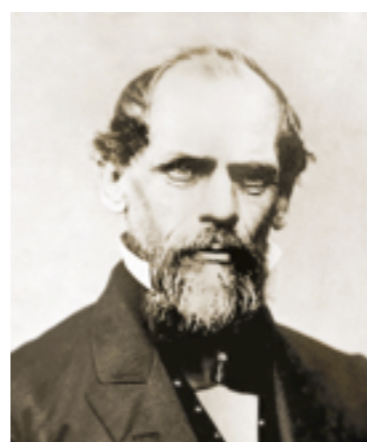
# Geometry of Filamentous Matter:



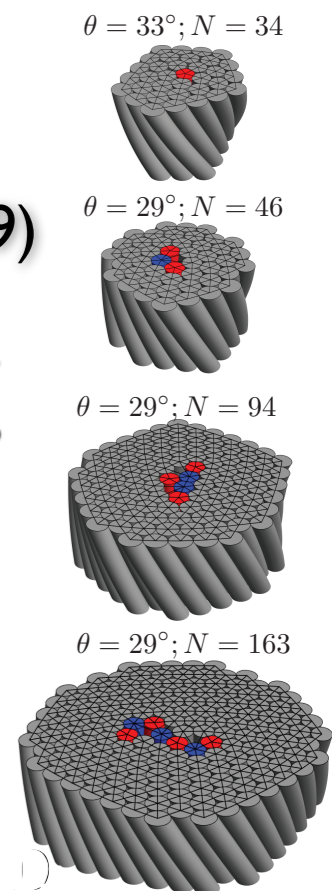
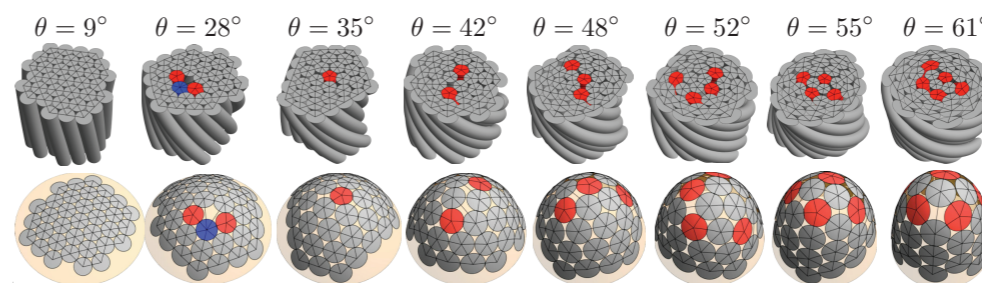
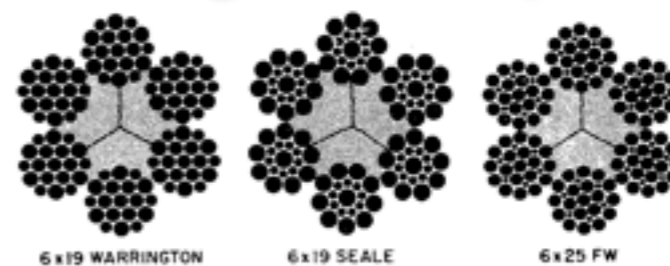
Optimal packing on spheres:  
**Thomson Problem** (1904)



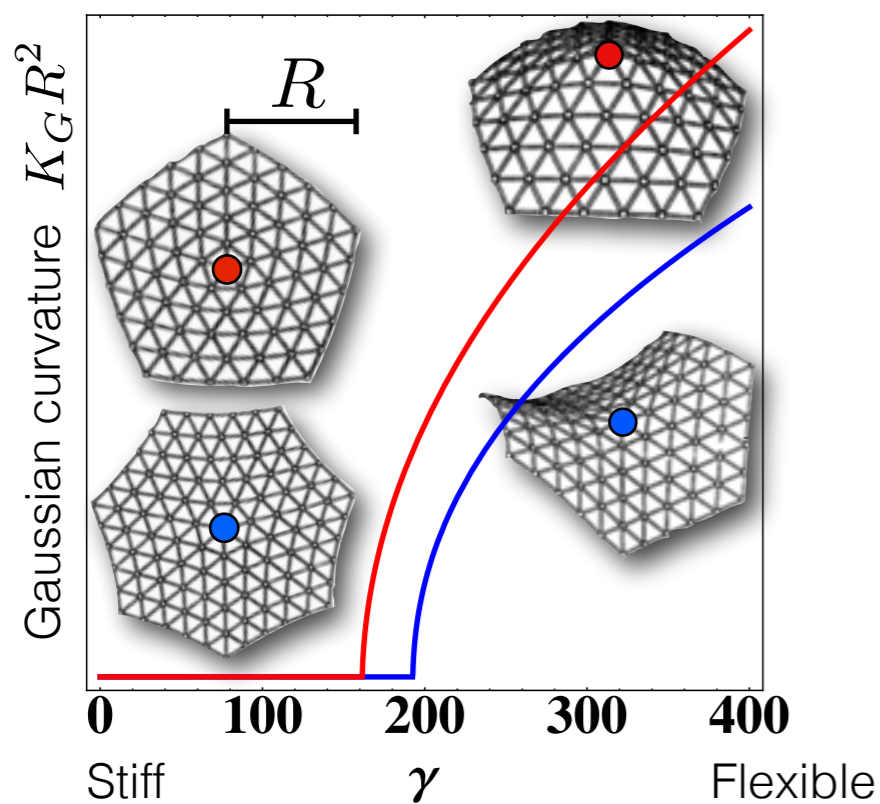
Wales, McKay & Altschuler, *PRB* (2009).



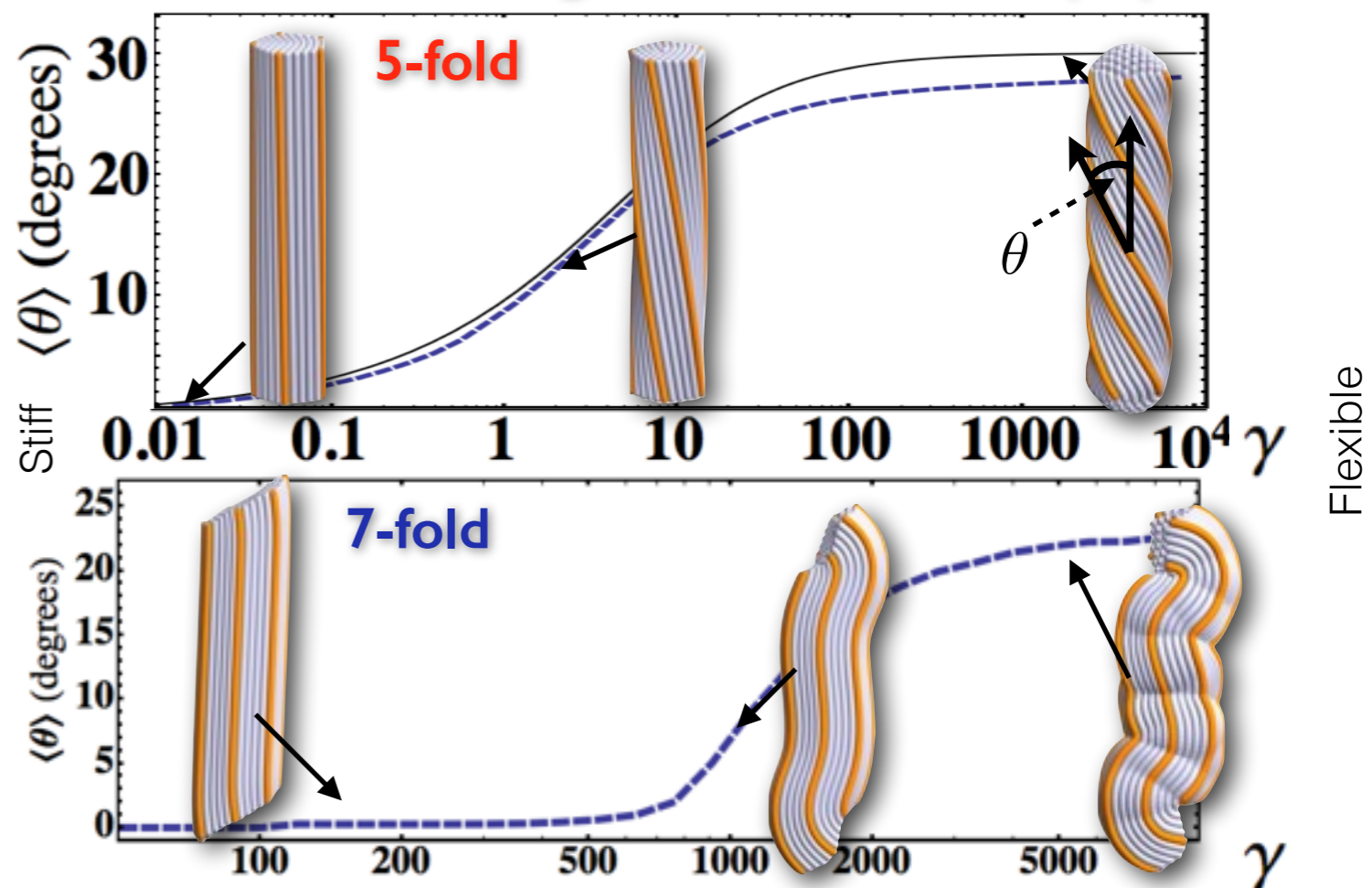
Optimal packing in ropes:  
**"Roebling Problem"** (~1849)



Defect-induced buckling of  
2D x-tals: Seung & Nelson (1988)



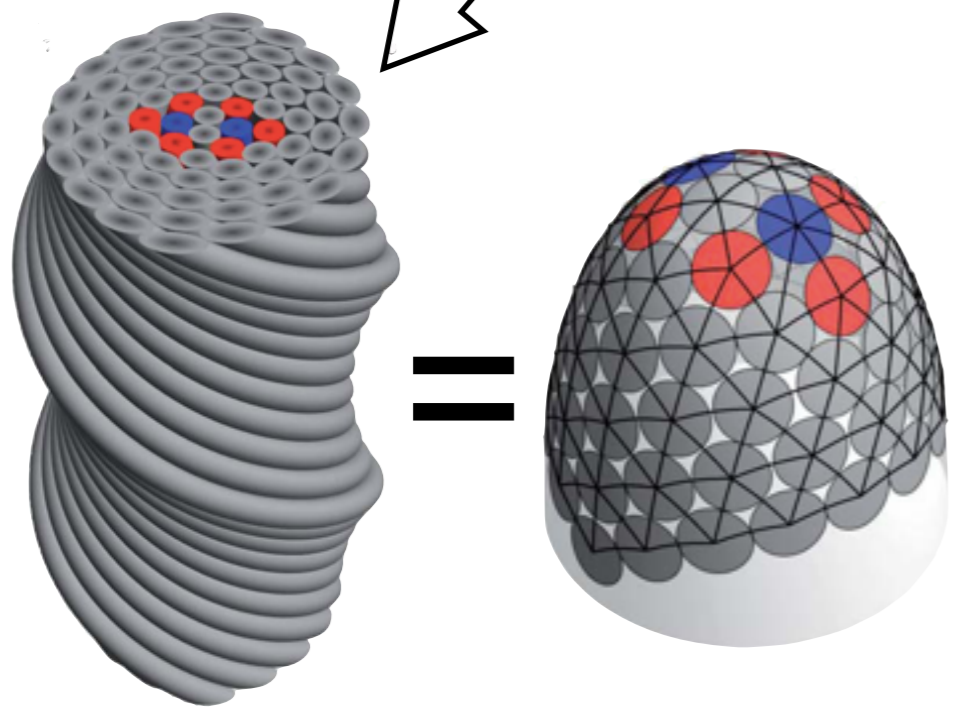
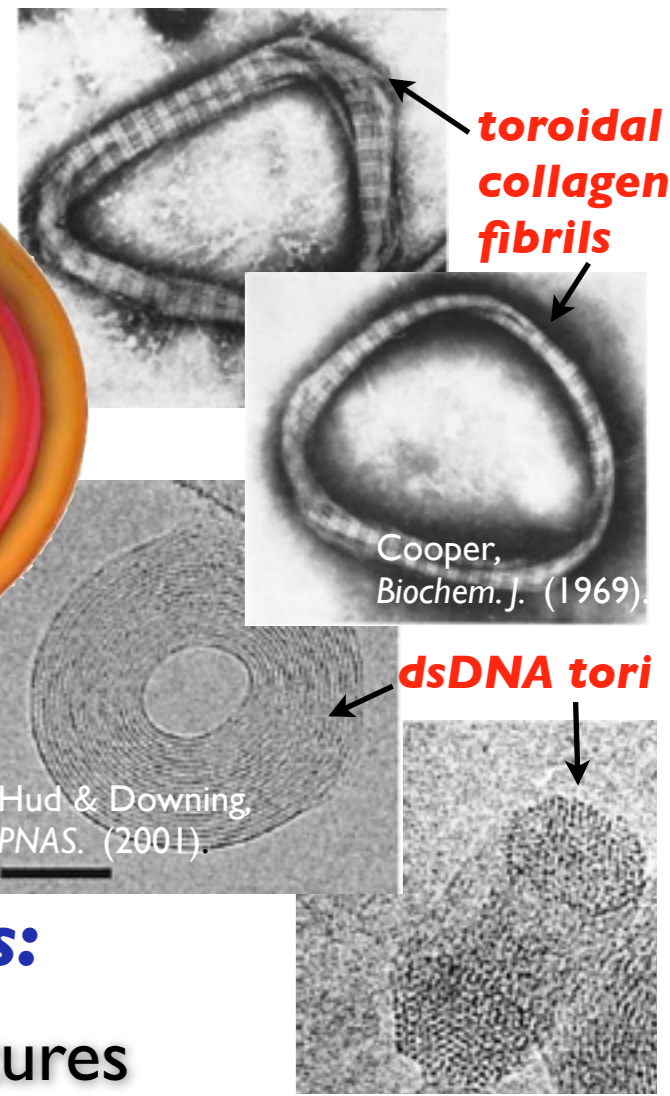
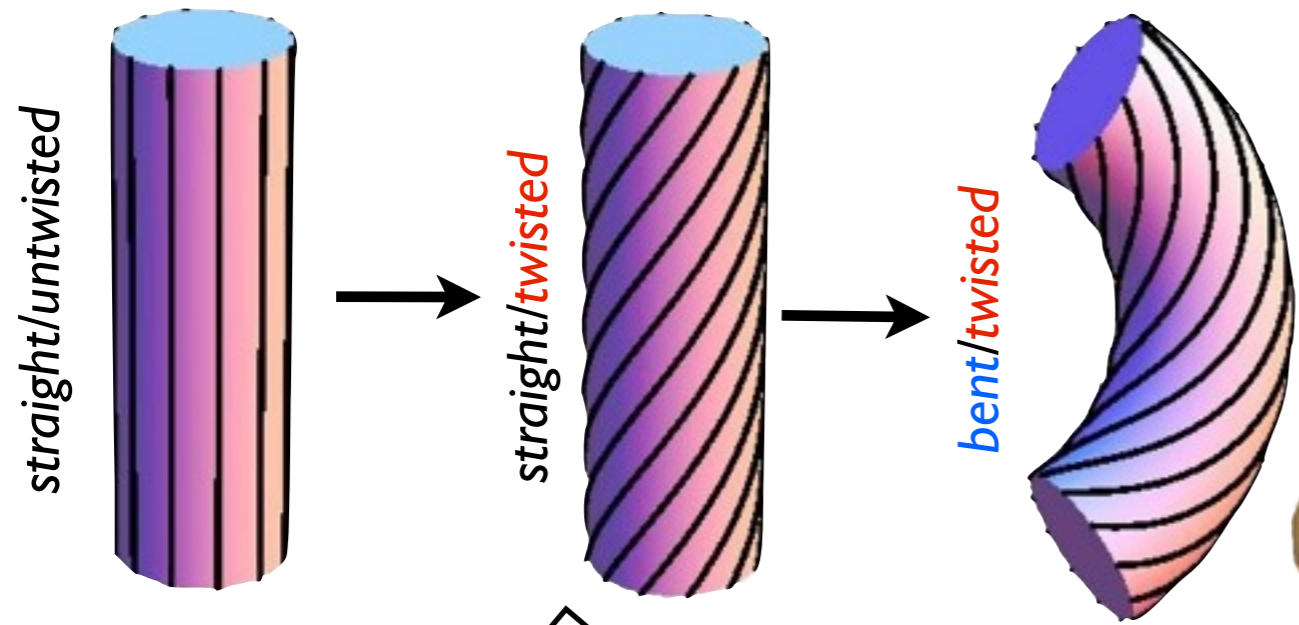
Defect-induced buckling of bundles: *Bruss in preparation*





# Packing filament beyond pure twist:

Prototypes of *bent* & *twisted* bundles:  
*twisted toroidal bundles*



screw symmetry  
 (straight/twisted)

equidistance filament  
 contact encoded in  
 single 2D surface

## “Cartography” of twisted toroidal bundles:

What are appropriate structures (embeddings) for “charting”/packing intrinsic inter-filament geometry?

How does metric geometry (or geometries) depend on bundle curvature?



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- Benny Davidovitch (UMass)

