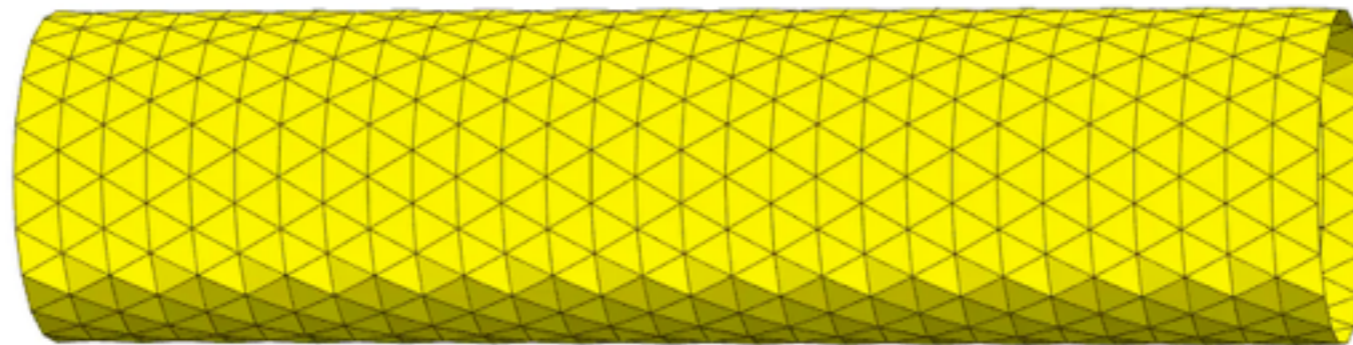


Plastic deformation of tubular crystals by dislocation glide



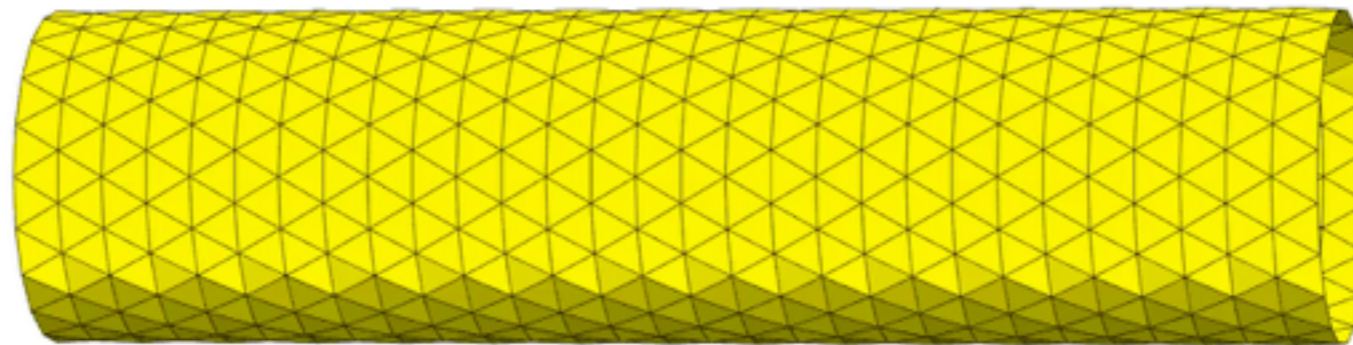
Daniel Beller, David Nelson

*Geometry, elasticity, fluctuations, and order
in 2D soft matter*

Kavli Institute for Theoretical Physics
January 14, 2016



Plastic deformation of tubular crystals by dislocation glide



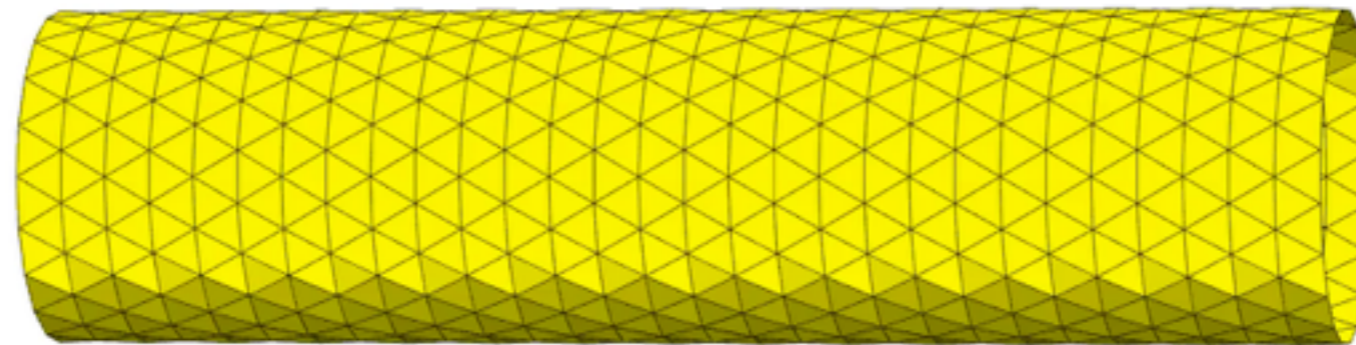
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Plastic deformation of tubular crystals by dislocation glide



Daniel Beller, David Nelson

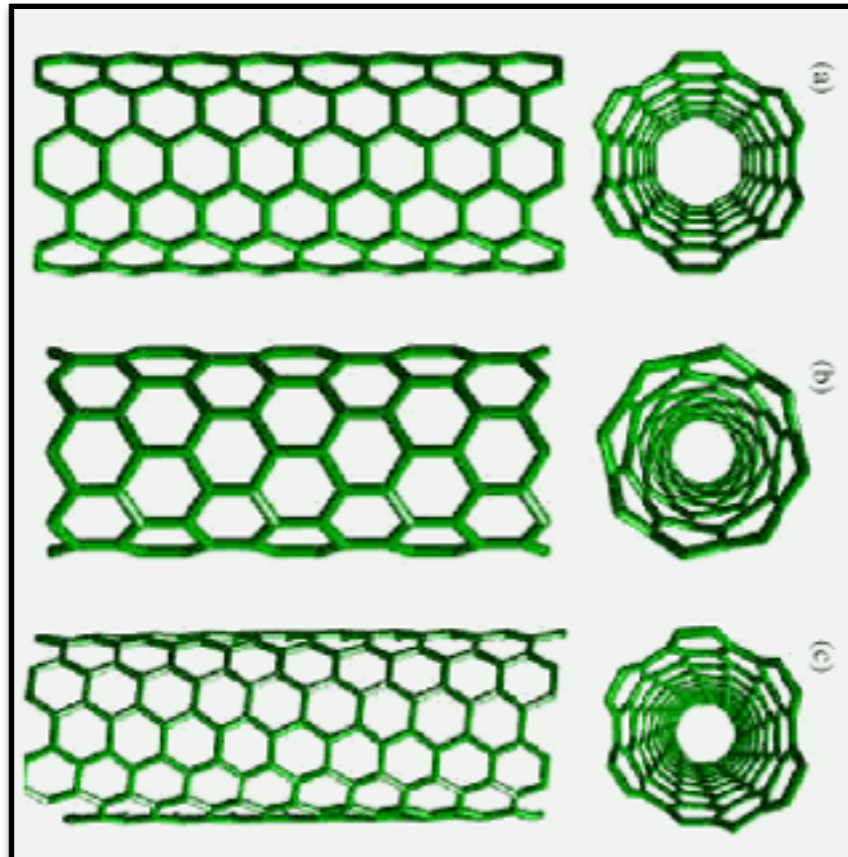
*Geometry, elasticity, fluctuations, and order
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Examples of tubular crystals

Single-walled carbon nanotubes



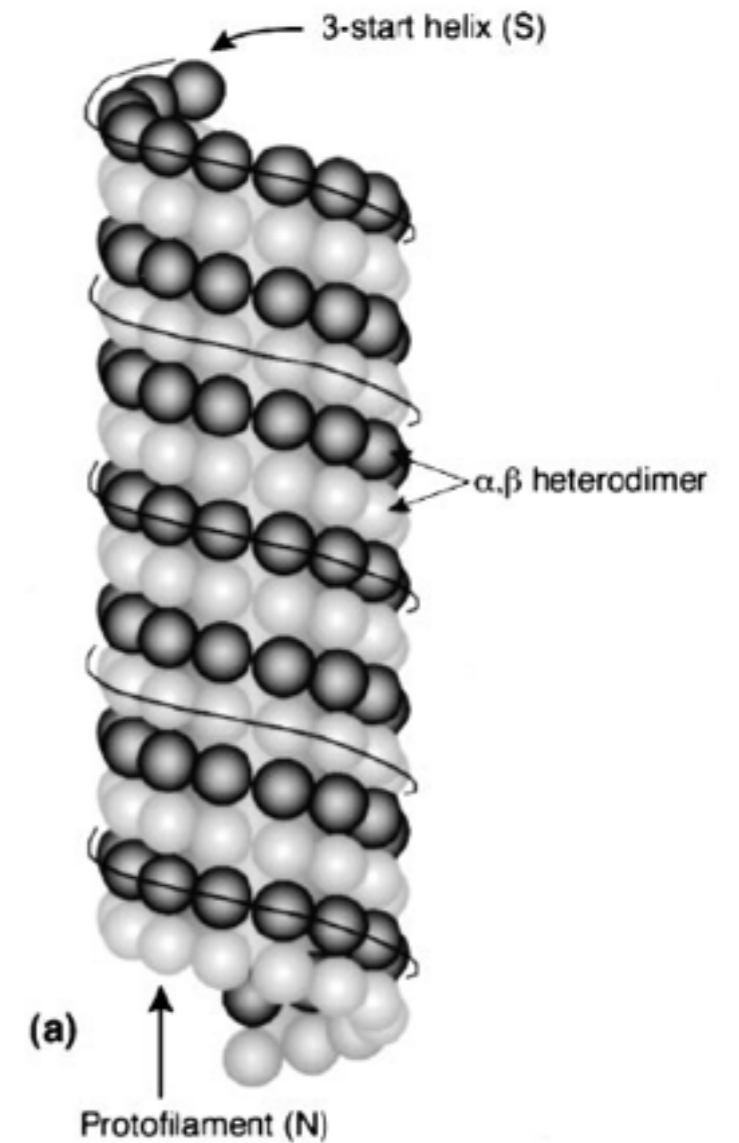
armchair

zigzag

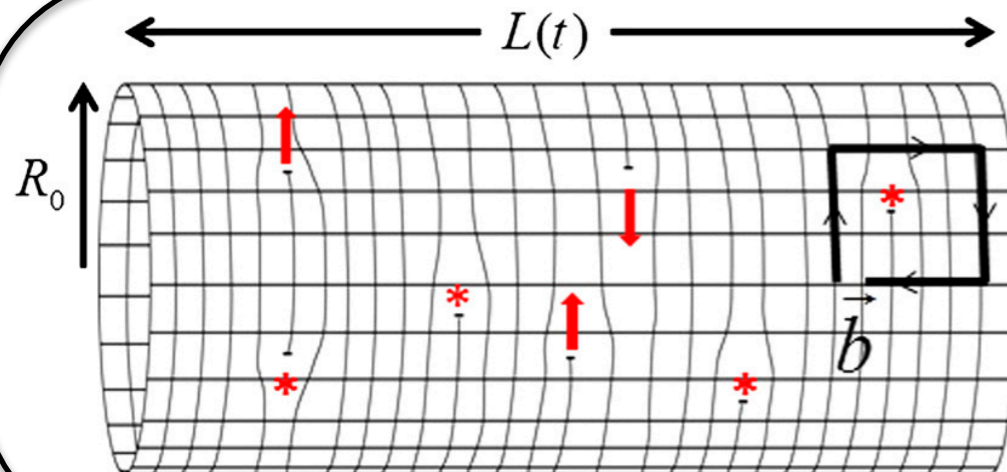
chiral

<http://education.mrsec.wisc.edu/nanoquest/carbon/>

Microtubules



Chrétien *et al.*, Eur Biophys J, 1998.

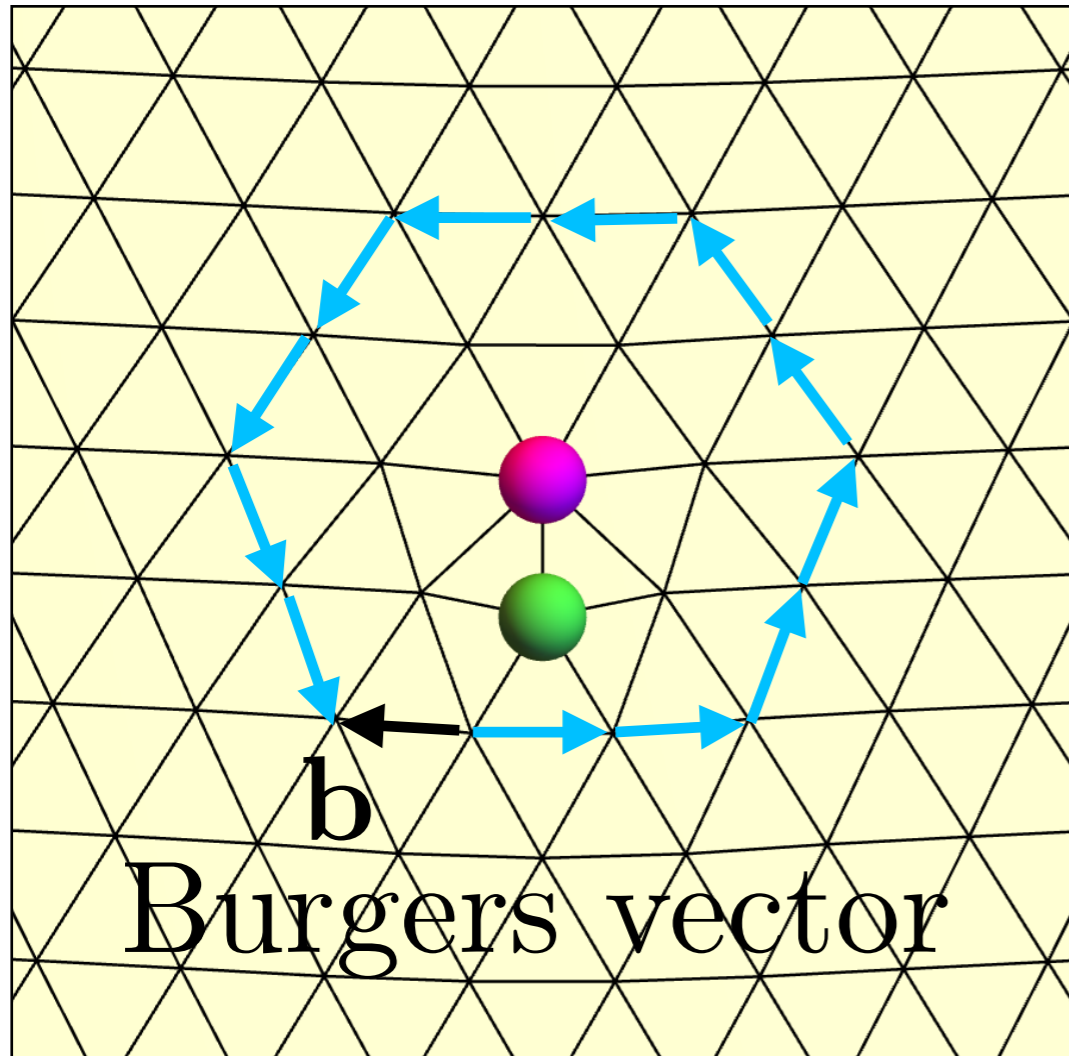


Bacterial cell wall (peptidoglycan mesh)

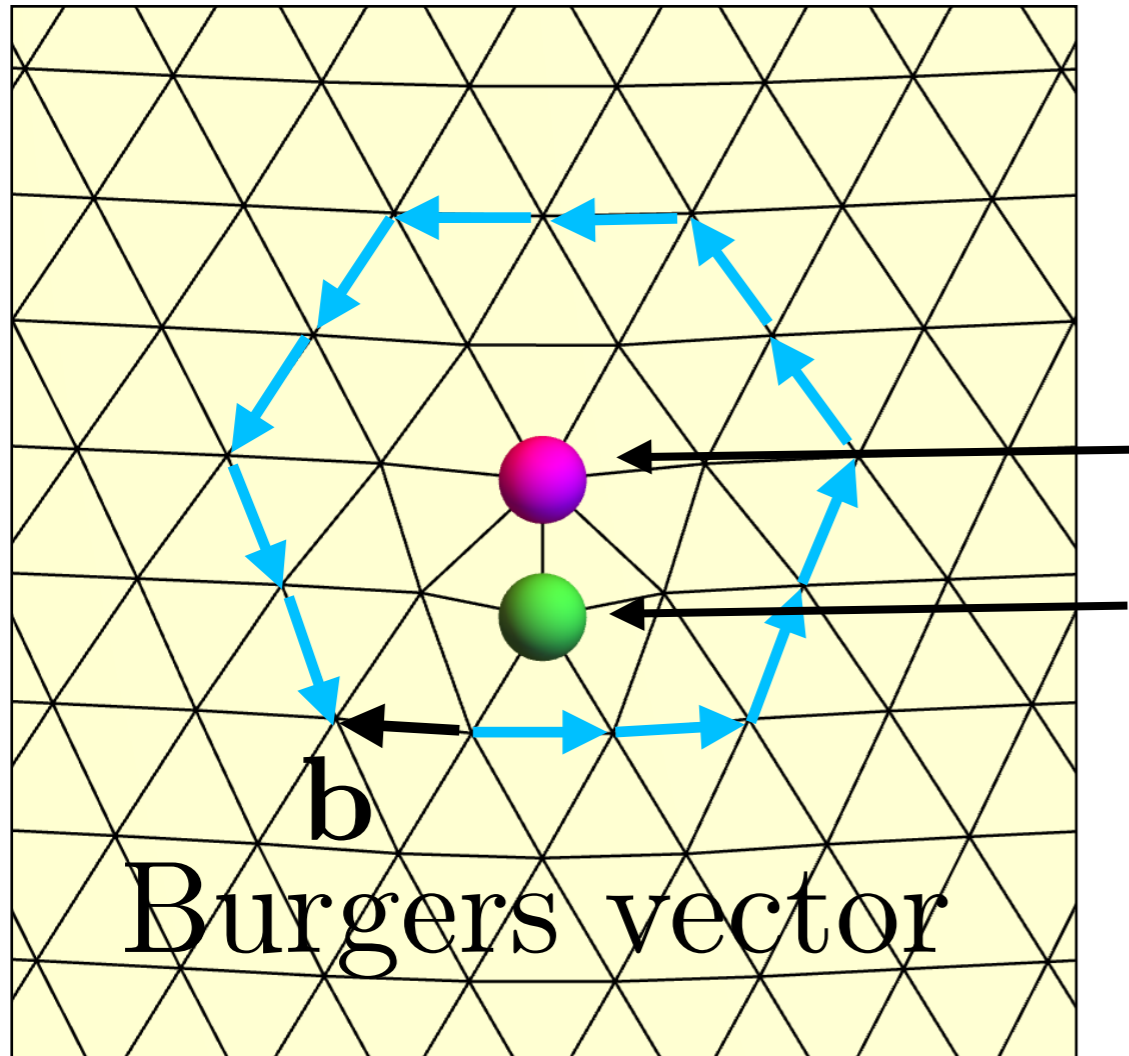
Amir & Nelson, "Dislocation-mediated growth of bacterial cell walls", PNAS 109:9833 (2012)

Each of these systems may contain dislocations...

Dislocation



Dislocation

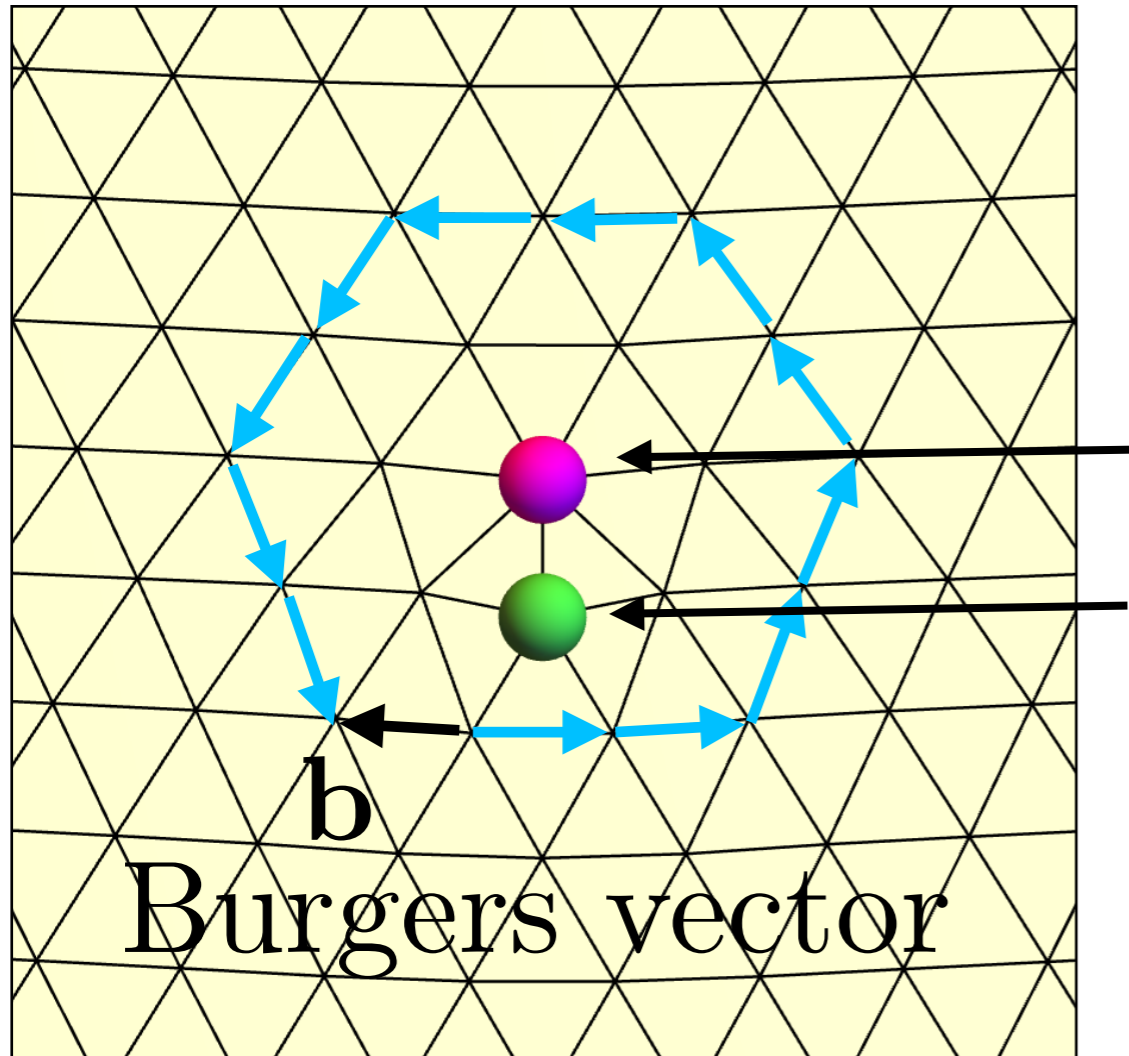


(In a triangular lattice)

7-fold disclination

5-fold disclination

Dislocation

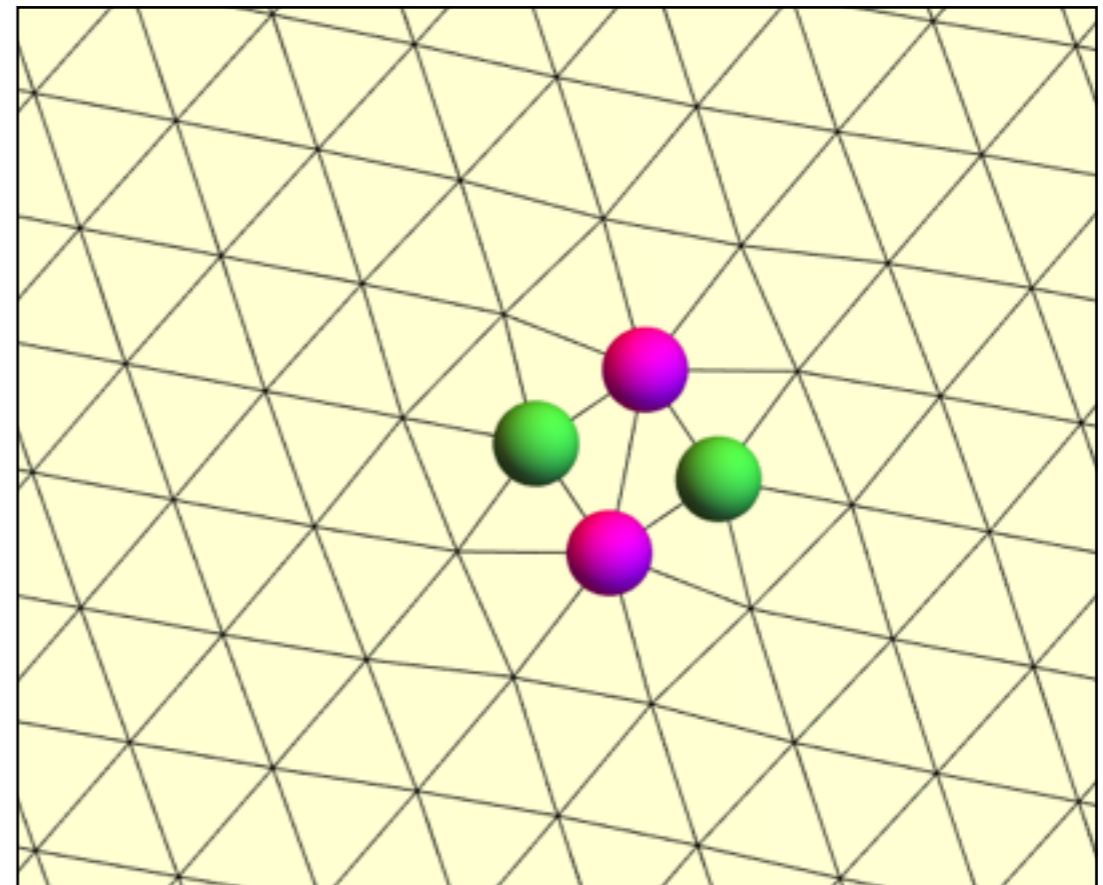


(In a triangular lattice)

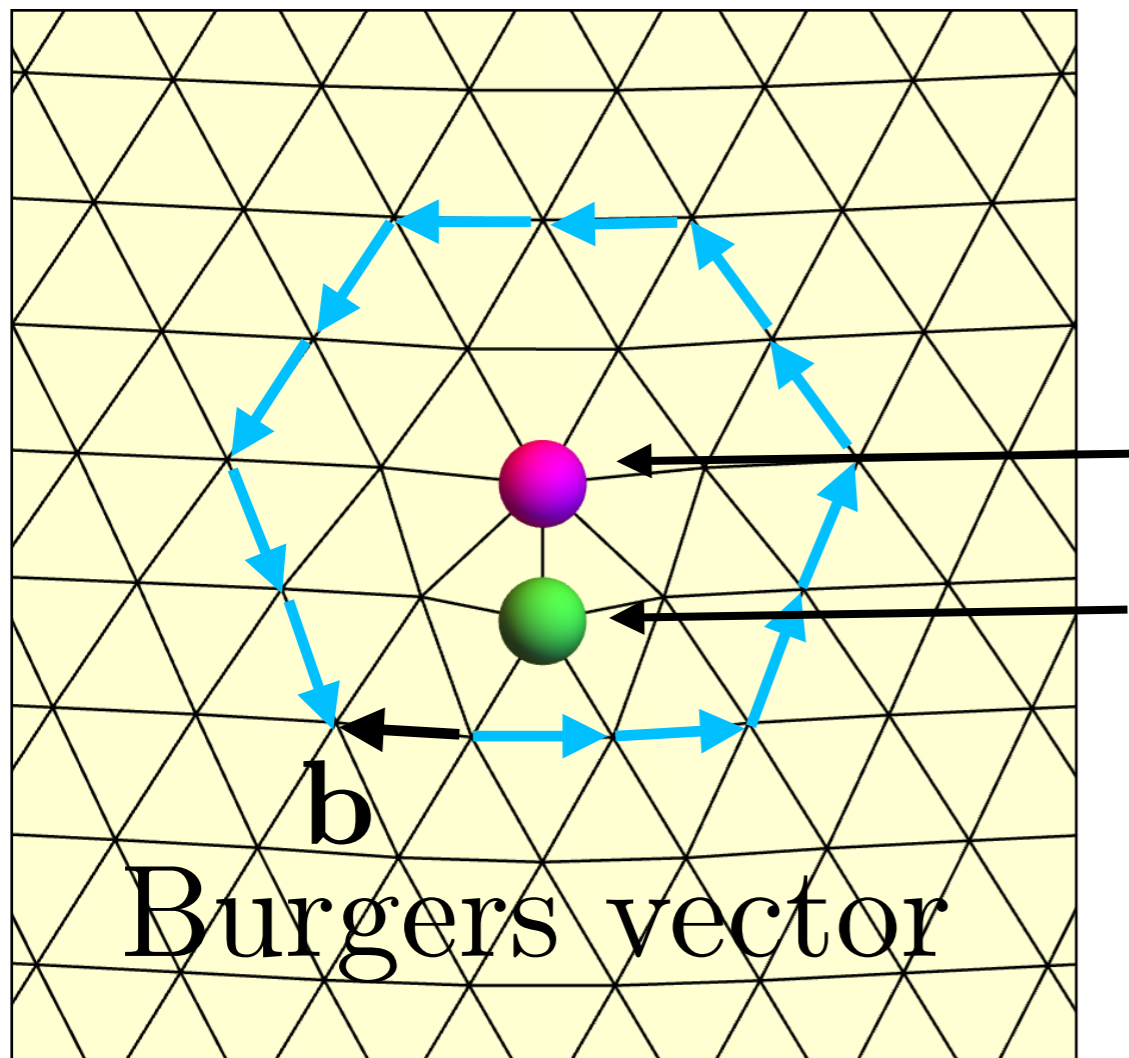
7-fold disclination

5-fold disclination

Dislocation pair



Dislocation

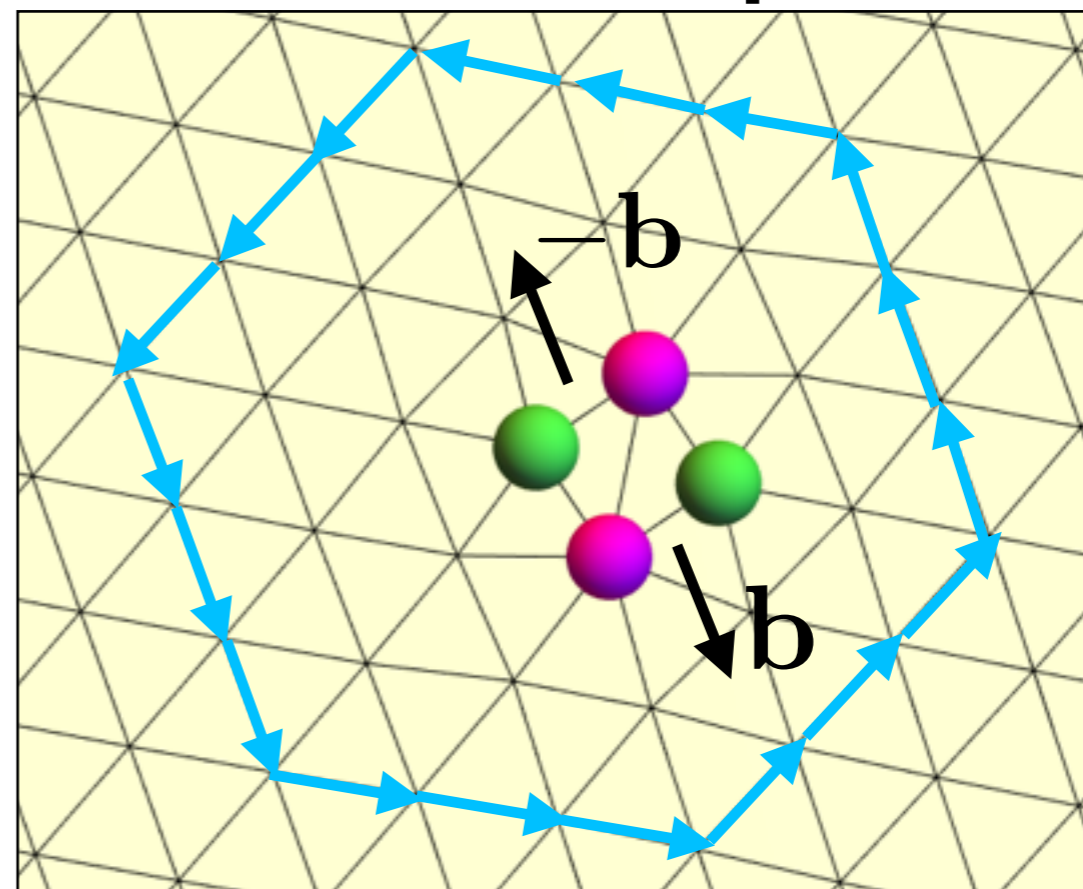


(In a triangular lattice)

7-fold disclination

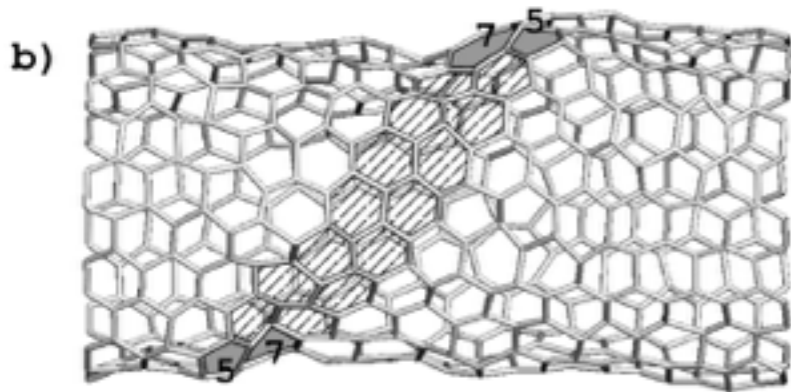
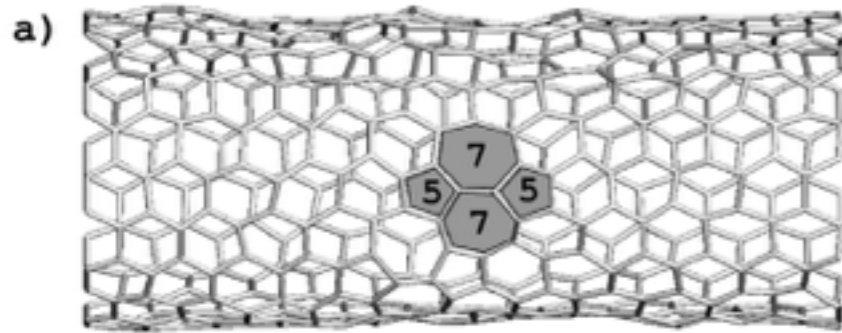
5-fold disclination

Dislocation pair

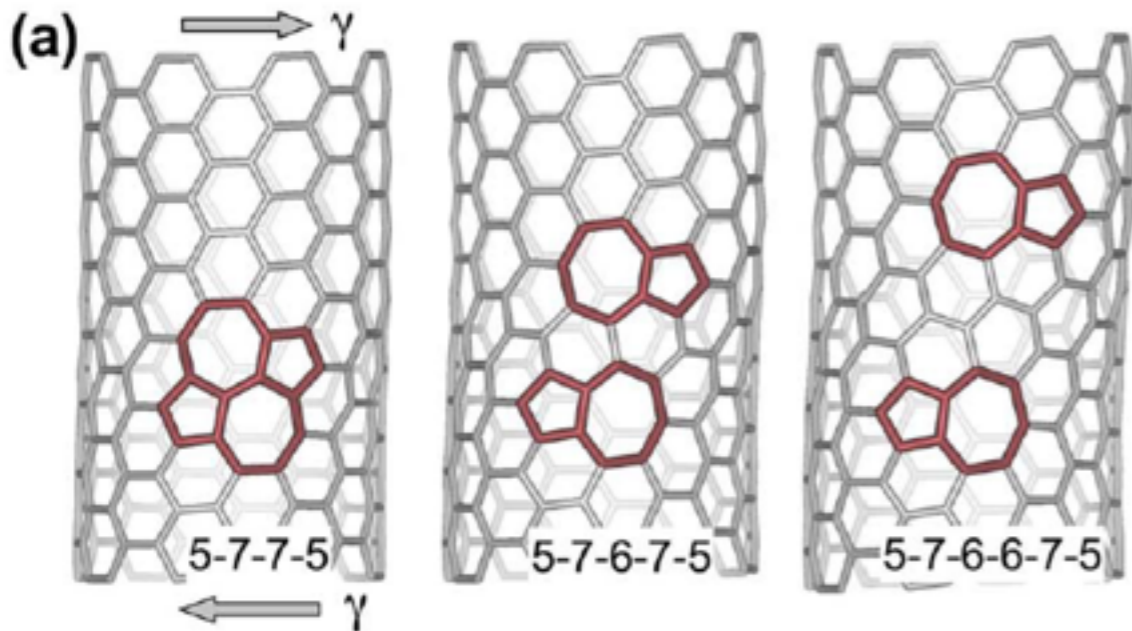


Single-walled carbon nanotubes plastically deform by dislocation motion at high temp

Simulation



Axial strain $\sim 10\%$
temperature = 3000 K
Nardelli et al., PRL 81:4656 (1998)

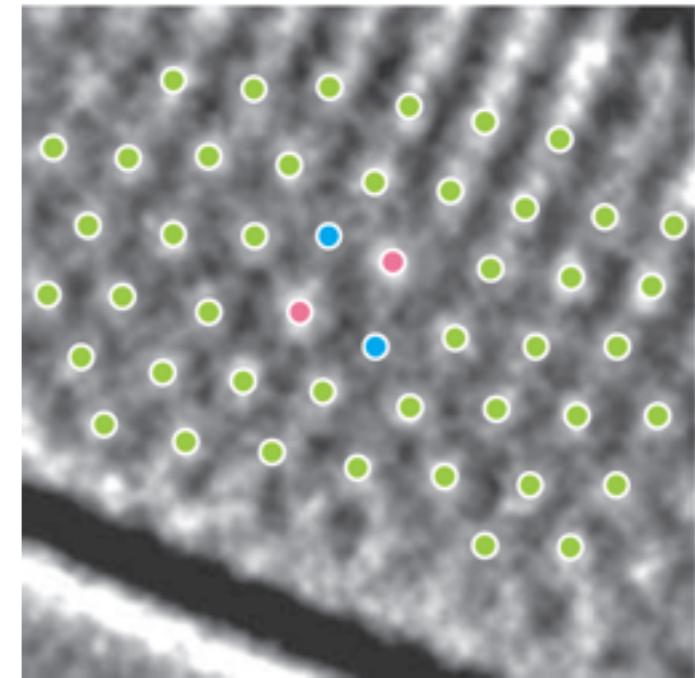


Torsional strain $\sim 10\%$

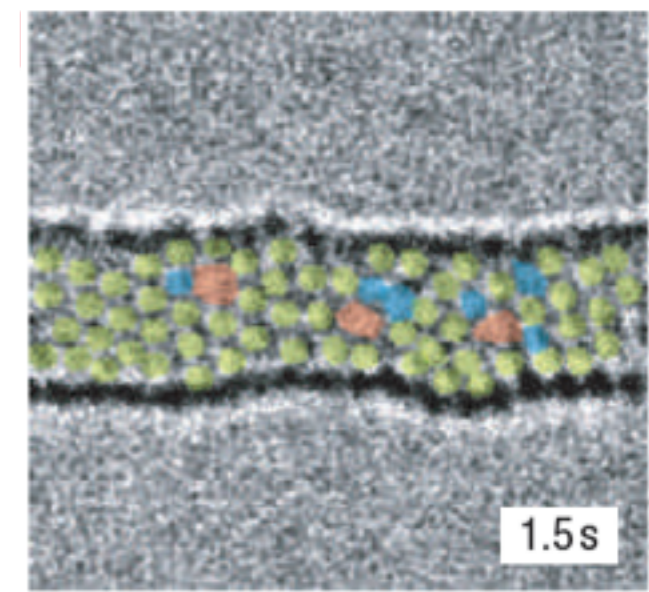
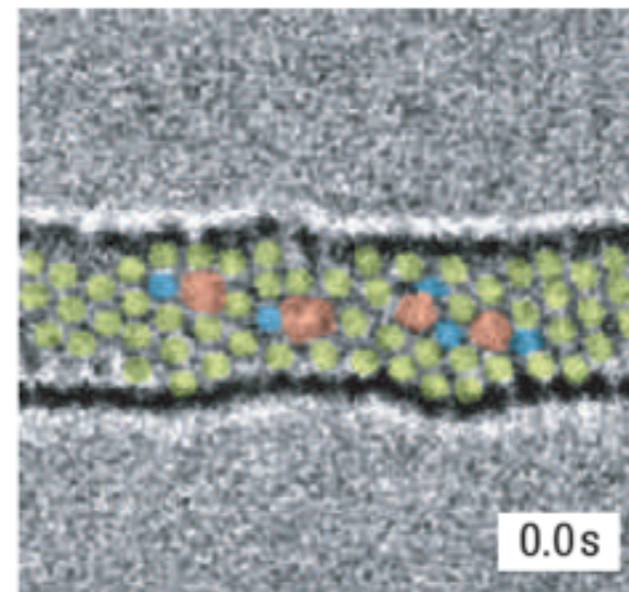
Zhang et al., J. Chem. Phys. 130:071101 (2009)

Experiment

Dislocation pairs found at $T = 2273$ K

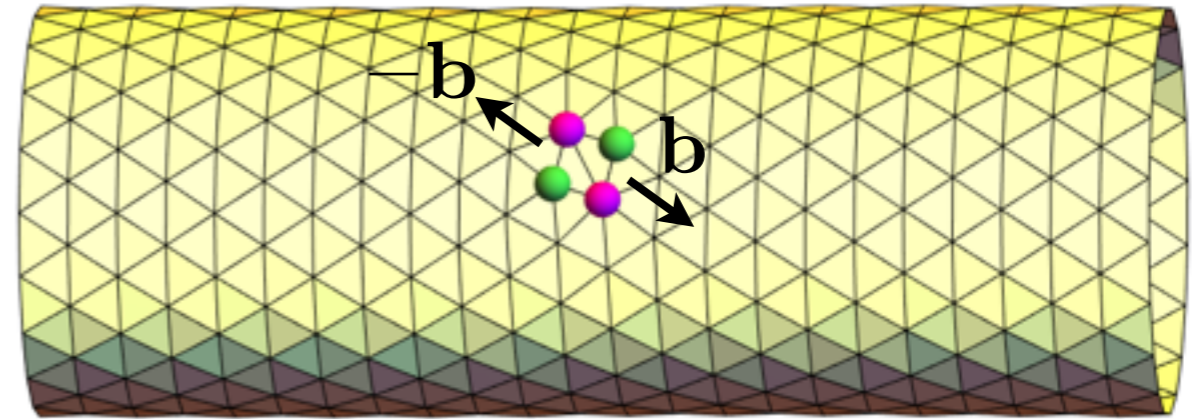


Dislocations migrate in presence of kink



Suenaga et al., Nature Nanotech. 2:358 (2007)

In this talk:
Dislocations in triangular
crystals on tubes



Plastic deformation of tubular crystals

- Background: Phyllotactic geometry of tubular crystals
- Mechanics of plastic deformation: Analytic predictions
- Numerical modeling
- Necks in tubes: Radius profiles near dislocations

Phyllotaxis (“leaf-arrangement”) in Botany

(Not the subject of this talk, but fascinating!)



sunflower

Pennybacker et al.,
Physica D 306:48 (2015)
^^^ a great review article!



aloe

Wikipedia

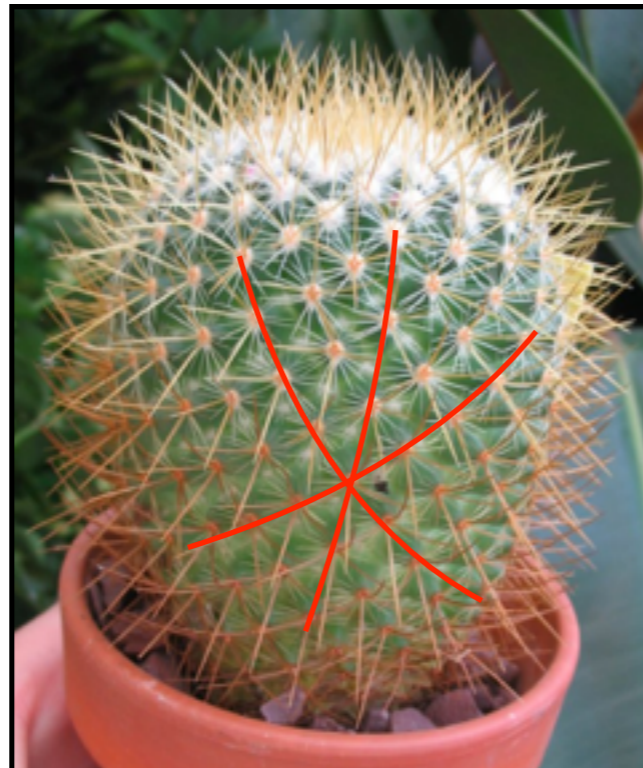


Romanesco broccoli

www.fourmilab.ch



Pineapple (D.A.B./Whole Foods)



Pincushion cactus

www.cactuslovers.com



Pine cone

Warren Photographic

Parastichies

Lattice lines →
Spirals or helices

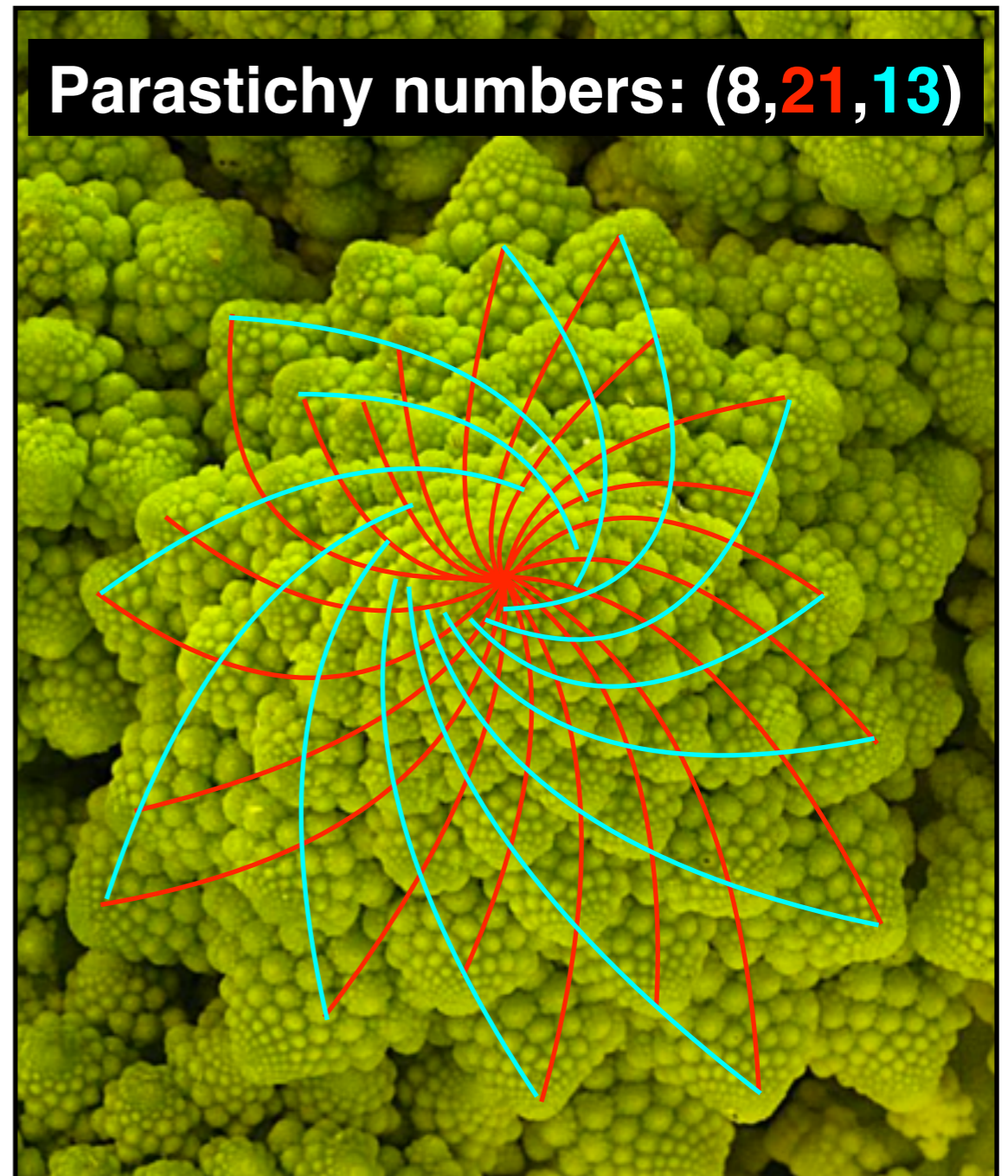
Phyllotaxis (“leaf-arrangement”) in Botany

(Not the subject of this talk, but fascinating!)

Phyllotactic packing is described by

parastichy numbers

= number of distinct parastichies in a
parastichy family

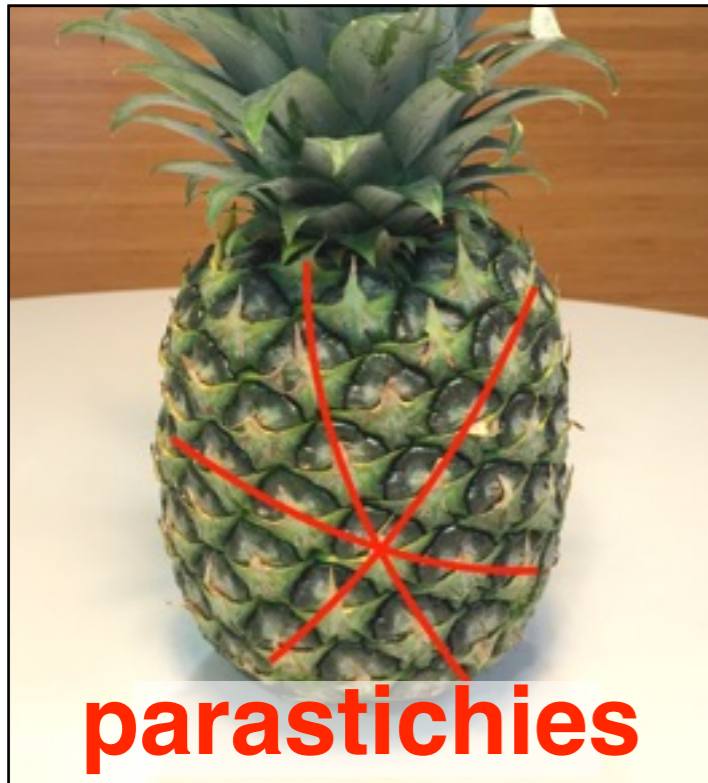


Romanesco broccoli

www.fourmilab.ch

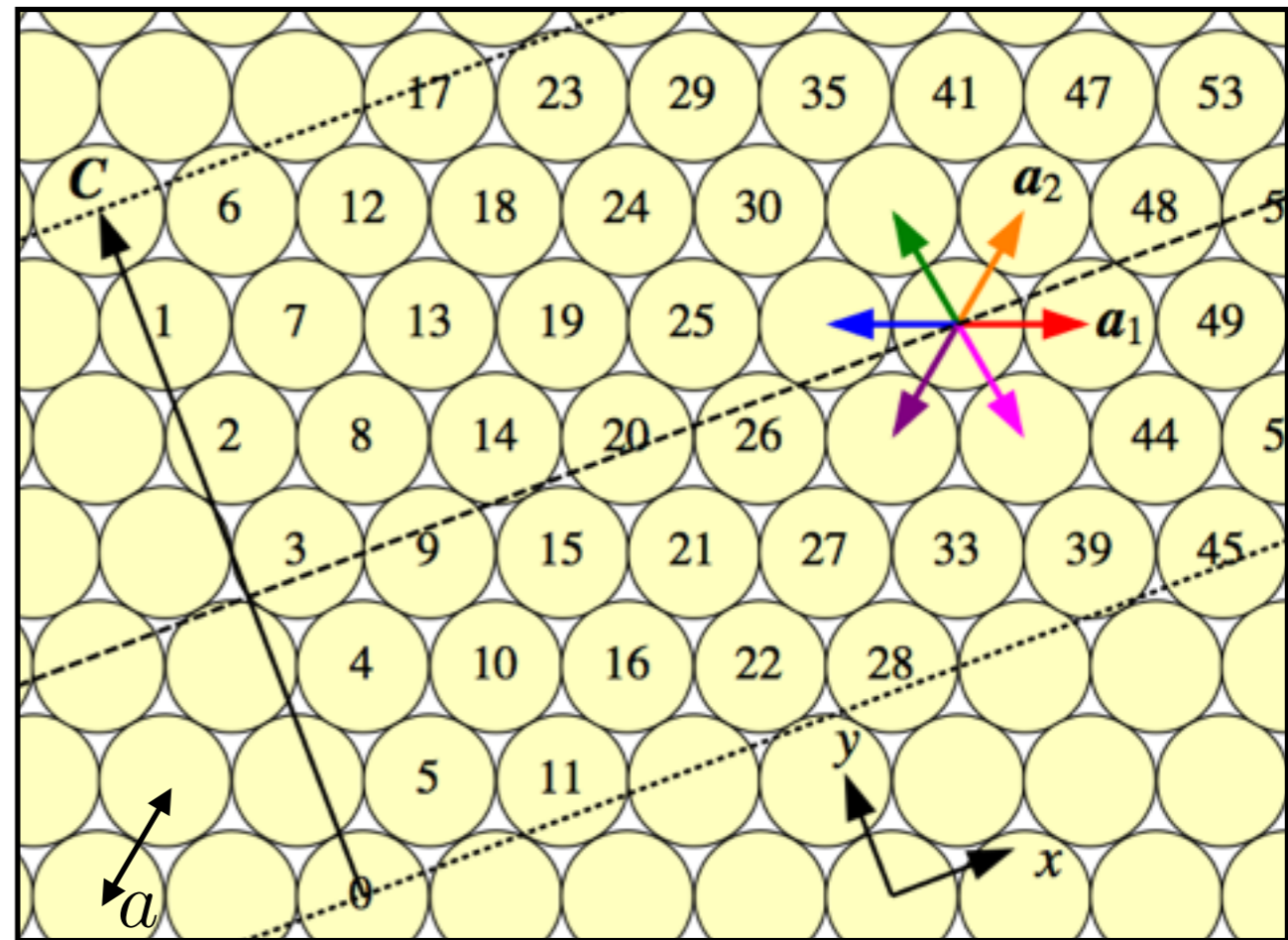
Phyllotaxis as the geometry of tubular crystals

Erickson, Science 181:705 (1973)

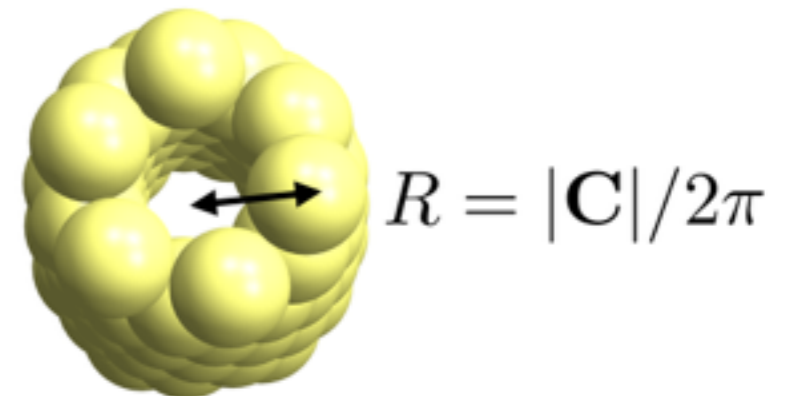
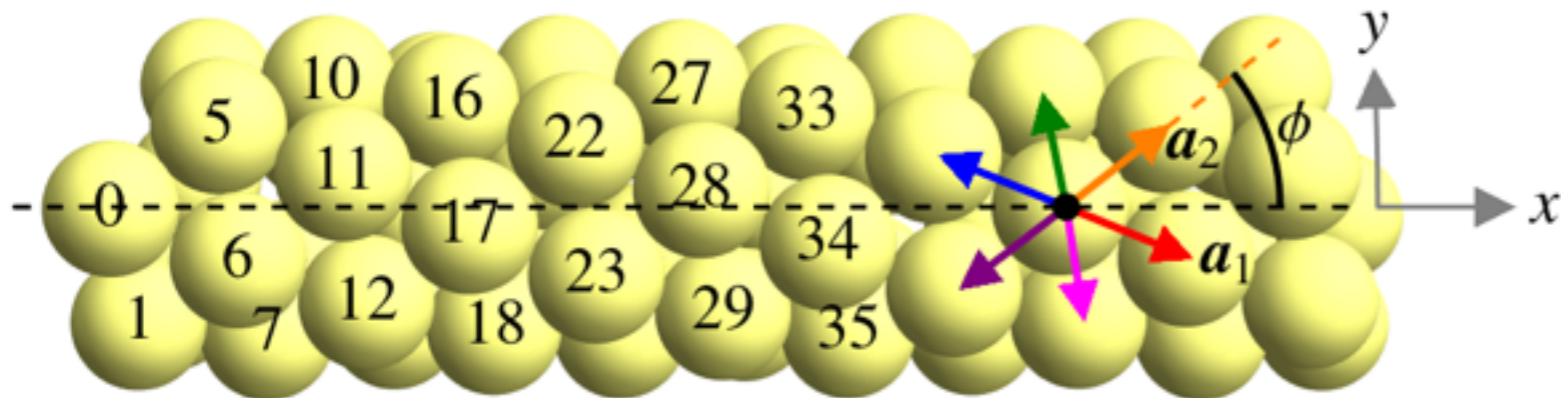


Circumference

$$\mathbf{C} = m\mathbf{a}_2 - n\mathbf{a}_1$$



parastichy numbers $(m, n) = (6, 5)$

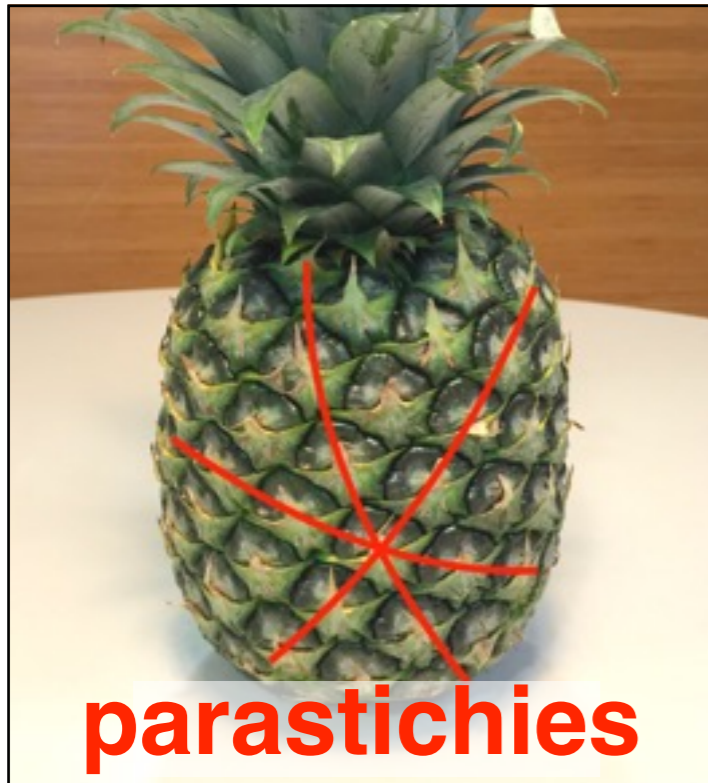


$$\tan \phi \approx \frac{2}{\sqrt{3}} \left(\frac{m}{n} - \frac{1}{2} \right) \quad R \approx \frac{1}{2\pi} |\mathbf{C}| = \frac{a}{2\pi} \sqrt{m^2 + n^2 - mn}$$

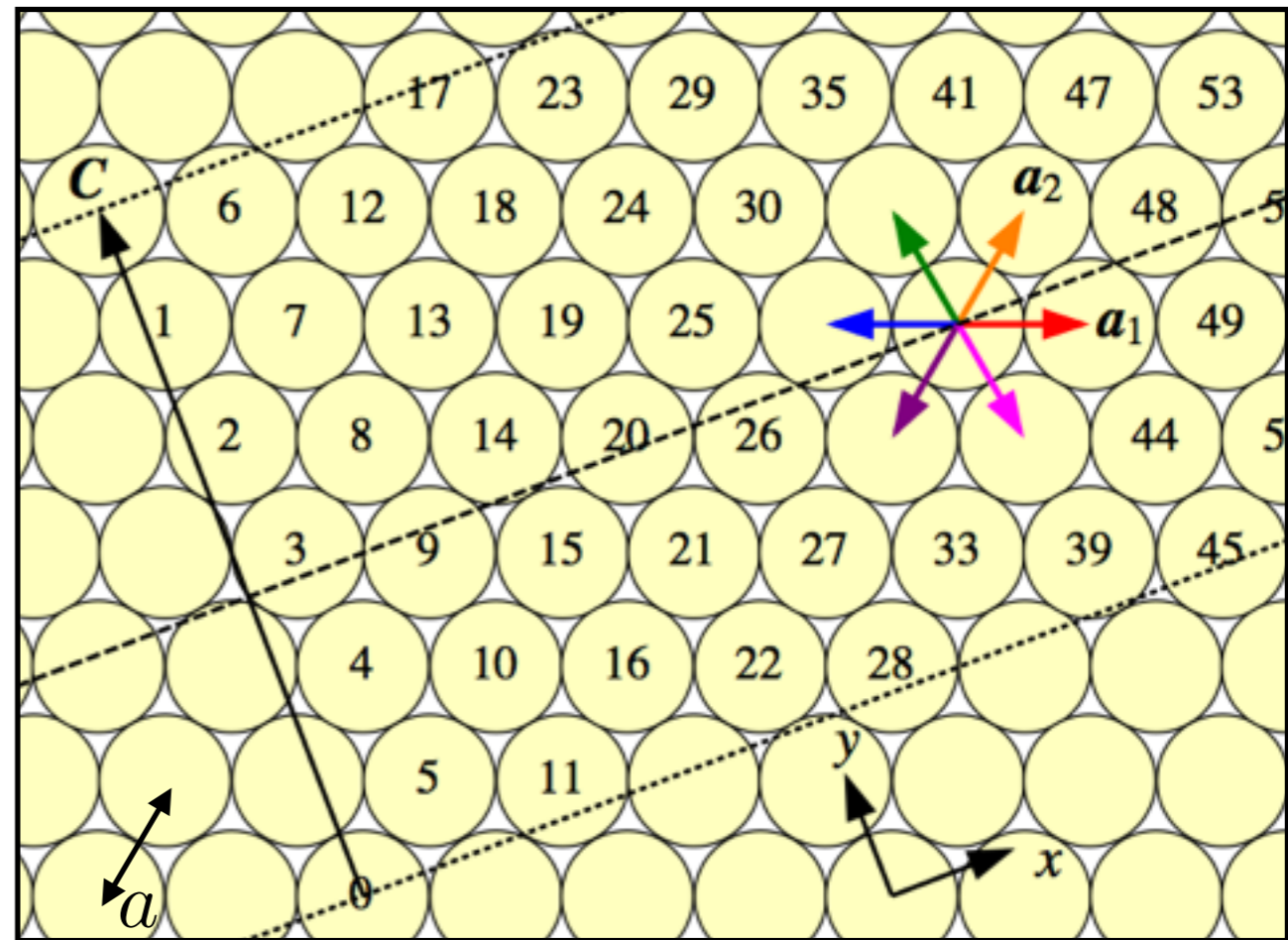
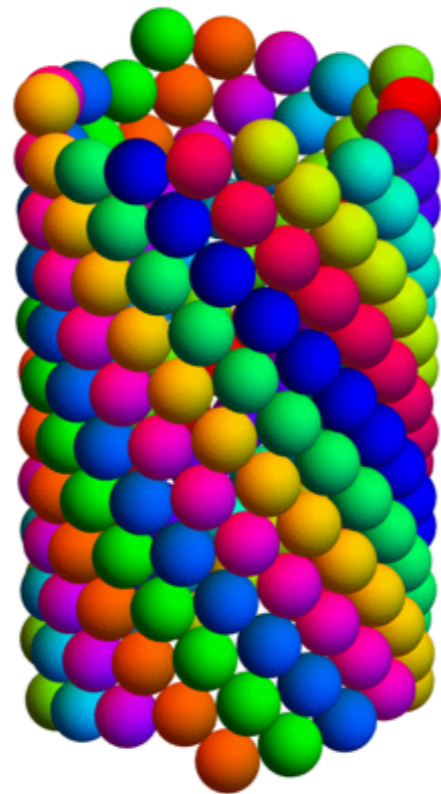
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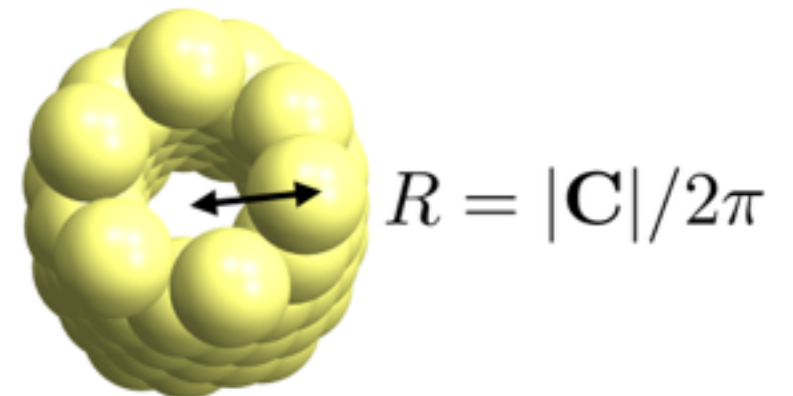
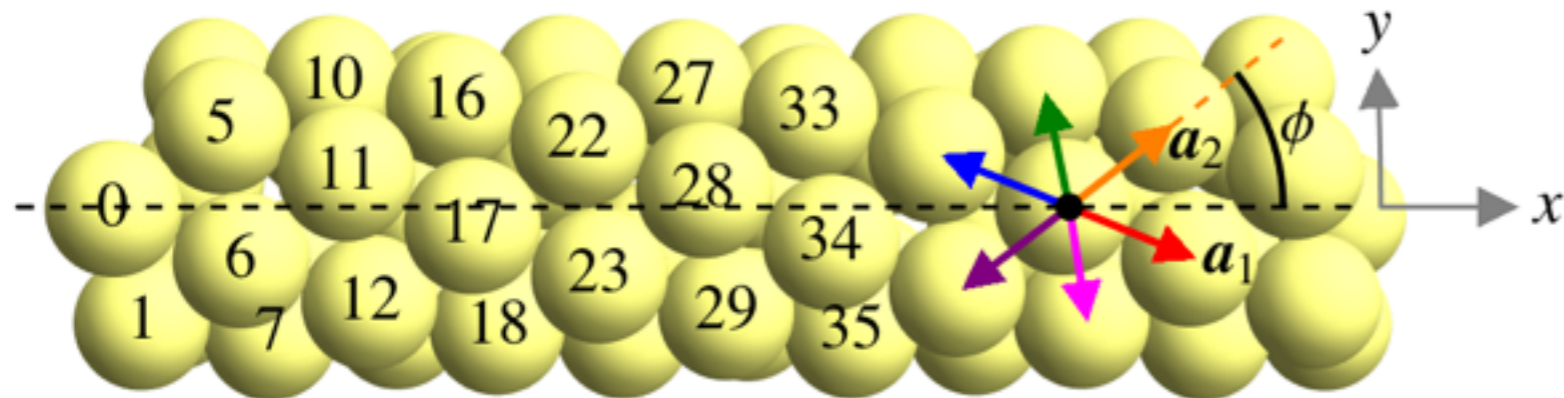


parastichies



parastichy numbers

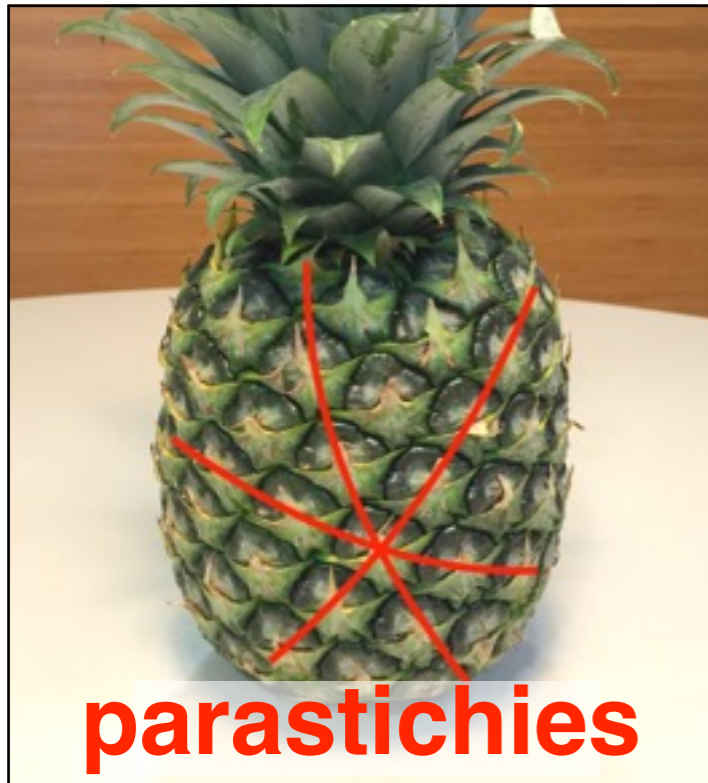
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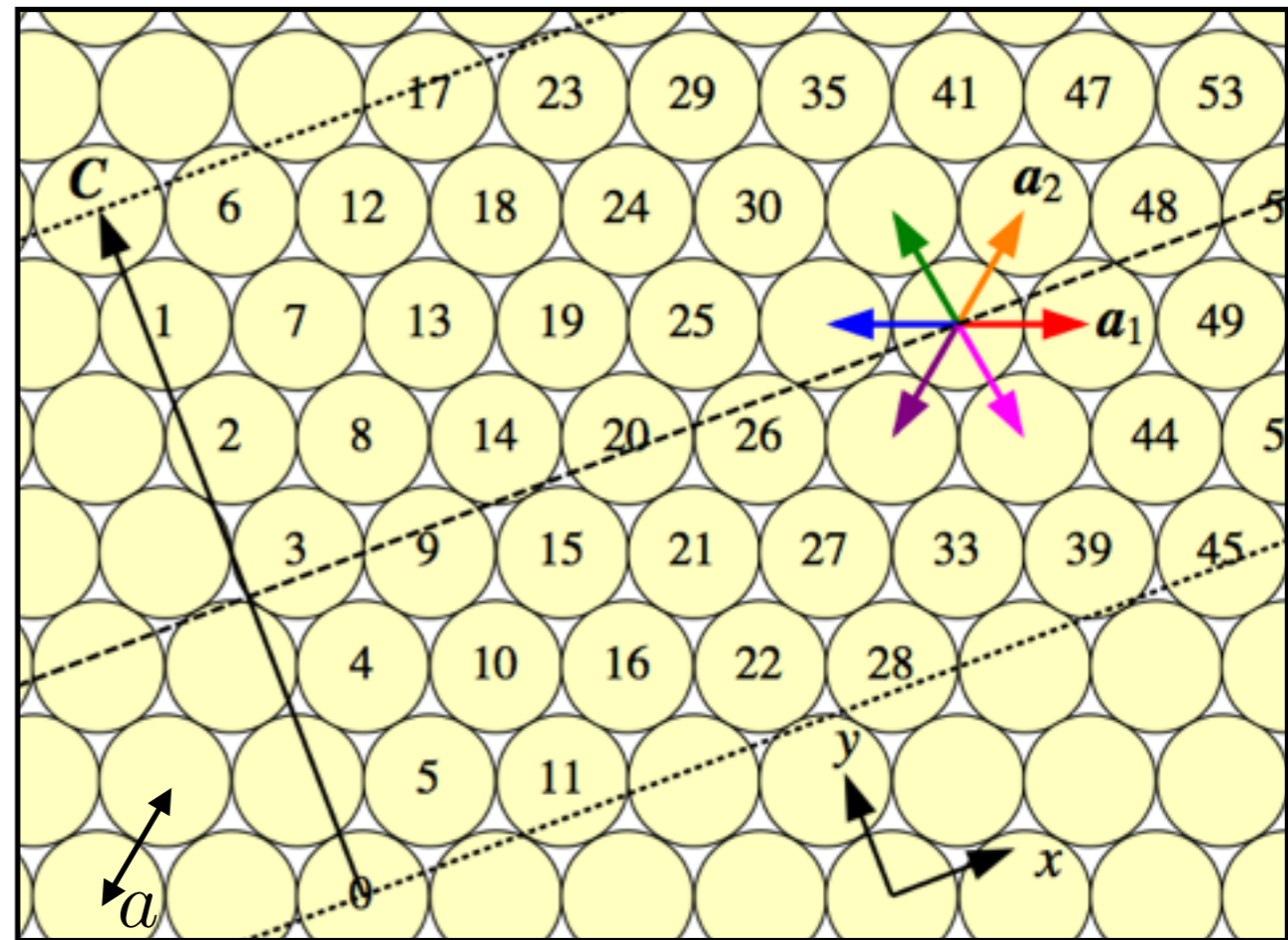
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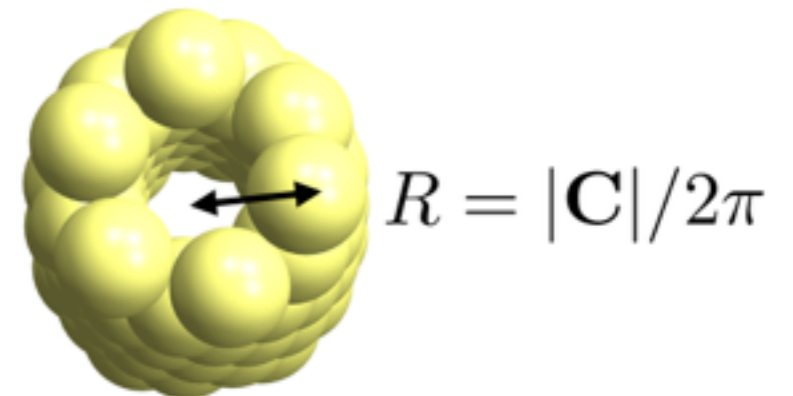
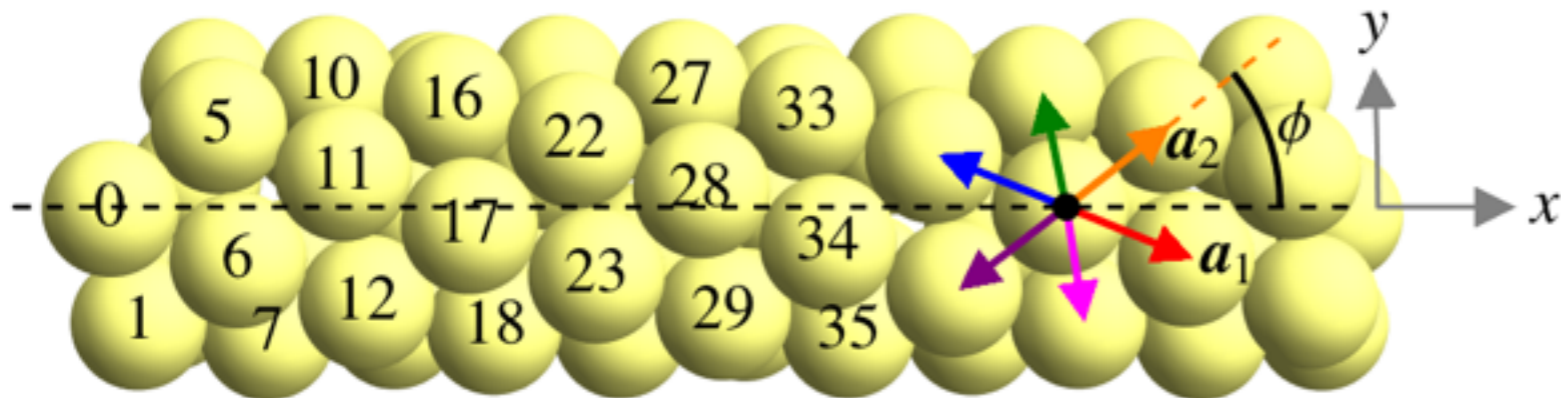


Circumference

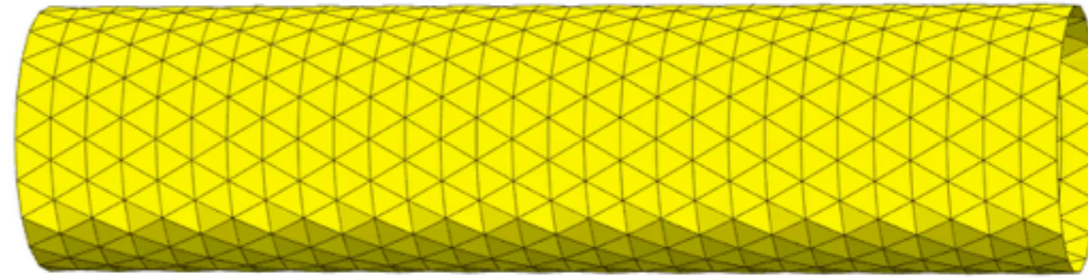
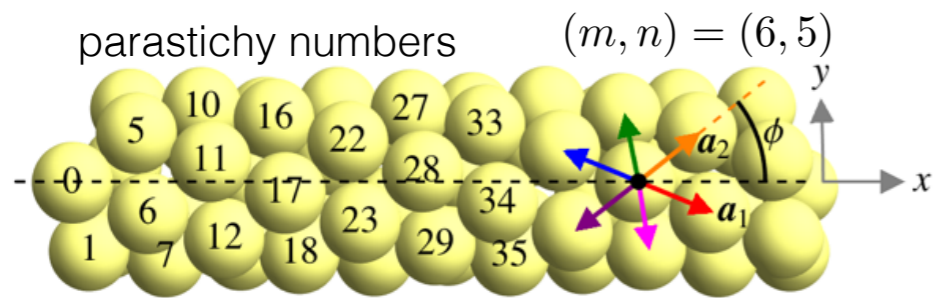
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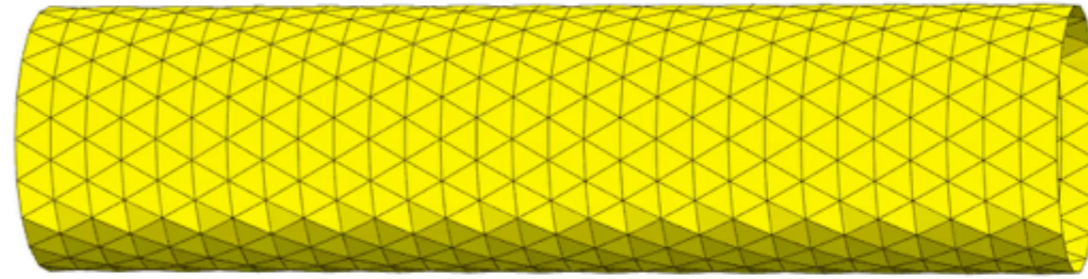
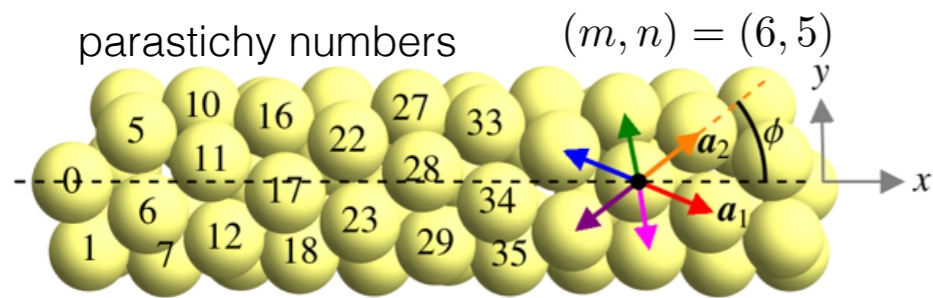


$$(m, n) = (20, 20) \rightarrow (20, 19)$$

This talk is about
Parastichy transitions, i.e., changes in (m, n) ,
 as plastic deformations
 accomplished by unbinding and separation of
 pairs of **dislocation defects**

Key questions

- How much stress is required to plastically deform a tubular crystal via dislocation motion?
- How do the softest plastic modes change the tube geometry?
- How well does continuum elasticity theory predict deformations in very small tubes?
- How does a crystals' bending modulus change the plastic deformation mechanics as compared with the plane?



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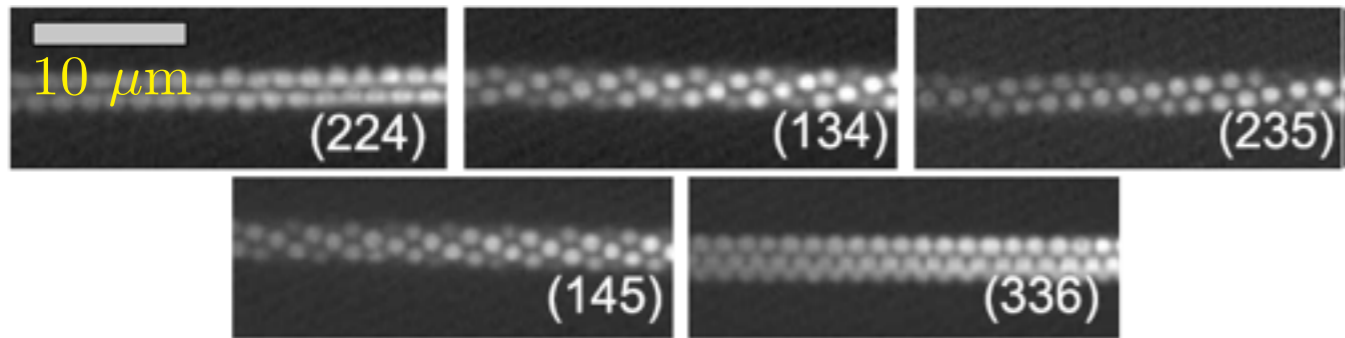
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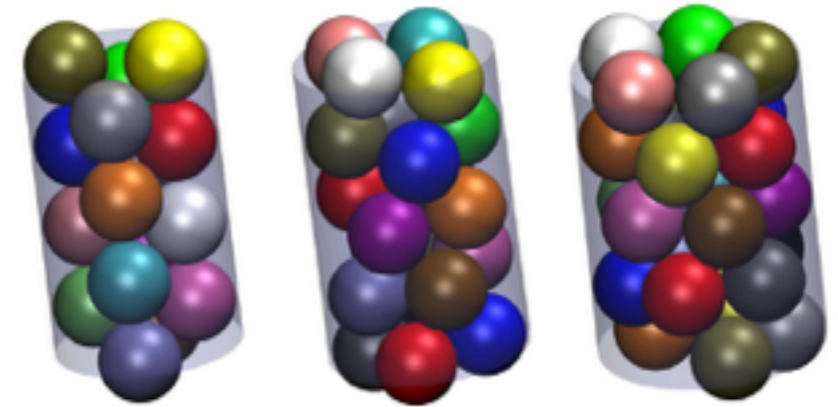
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Phyllotactic packings on cylinders of *fixed radius*: Recent work

Colloidal spheres in capillaries



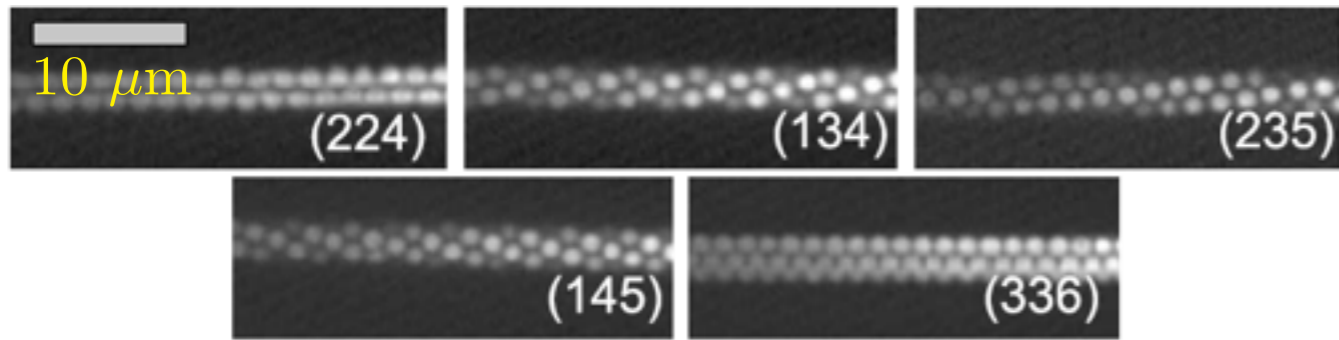
Lohr et al., PRE 81:040401 (2010)



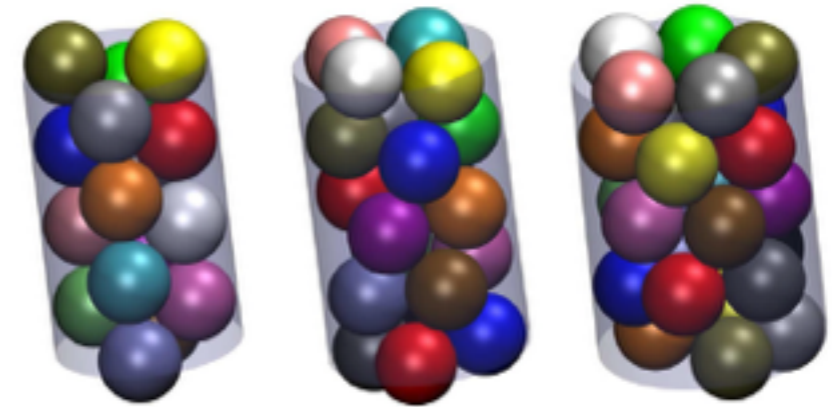
Mughal et al., PRL 106:115704 (2011)

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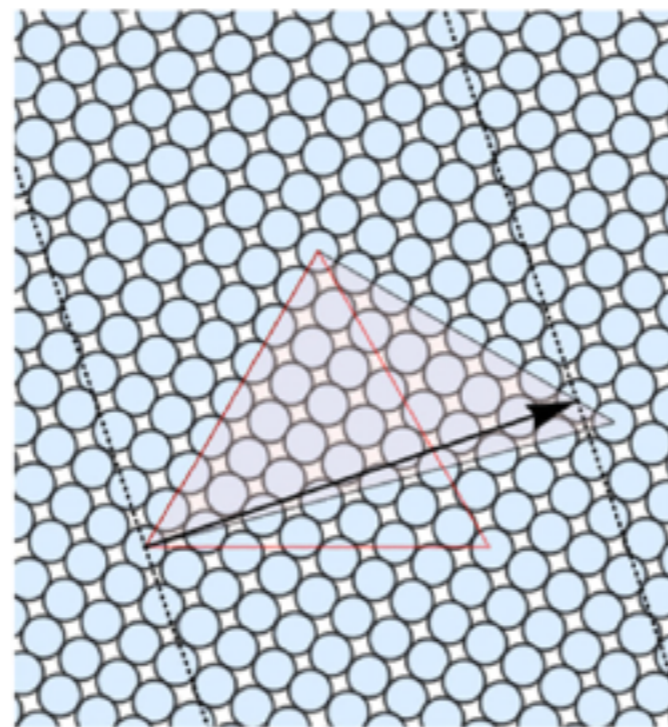
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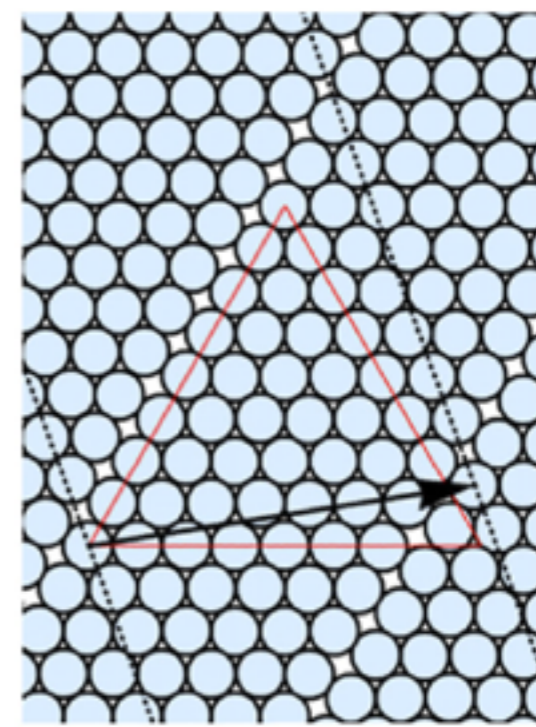
Mughal et al., PRL 106:115704 (2011)

What happens if the cylinder radius is incommensurate with any perfect phyllotactic packing?

Mughal and Weaire,
PRE 89:042307 (2014)



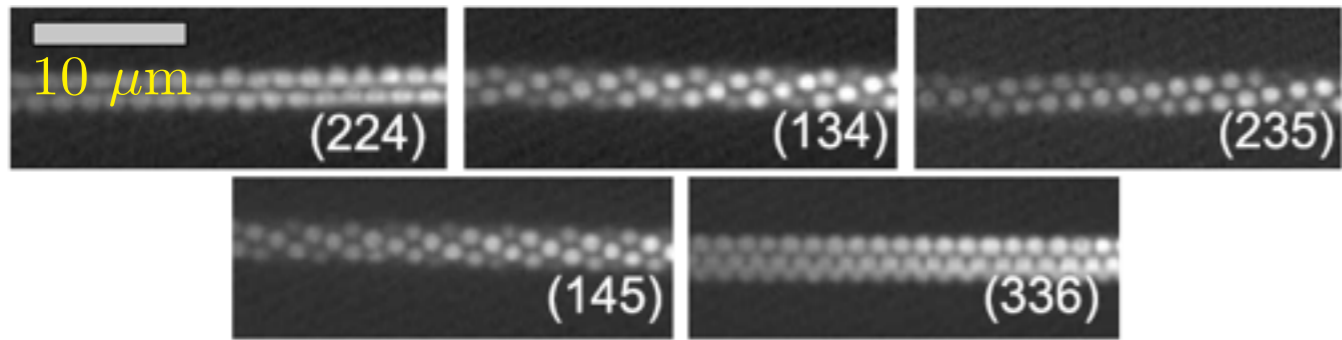
Rhombic (or "oblique") lattice



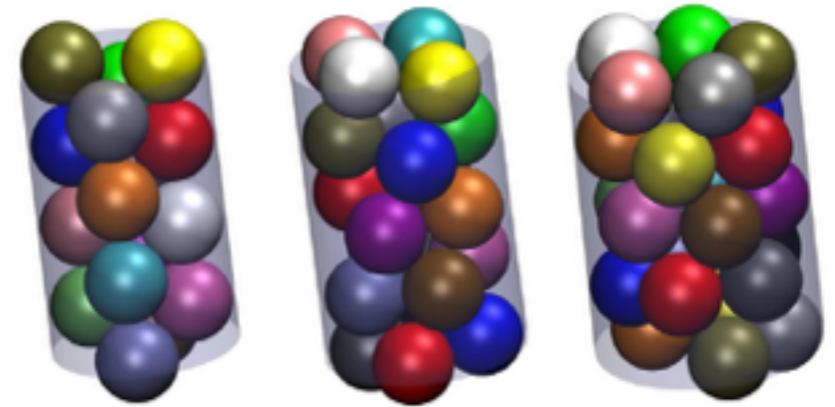
Helical "line-slip" defects in a triangular lattice

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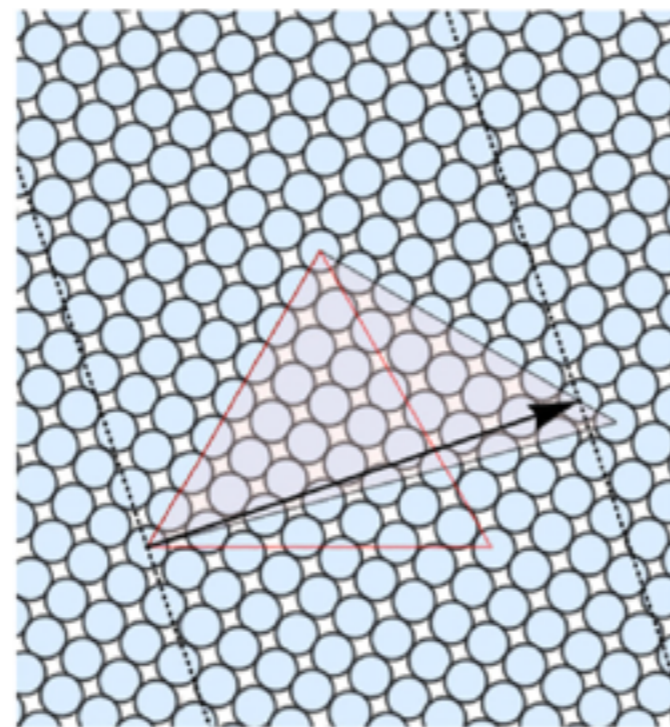
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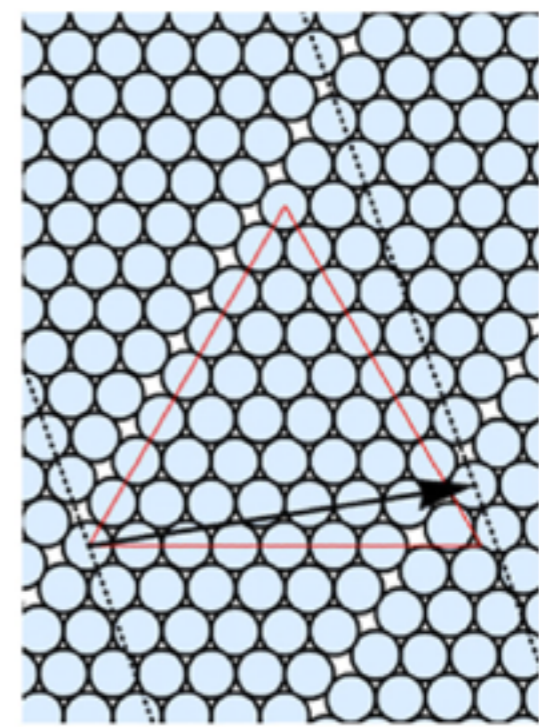
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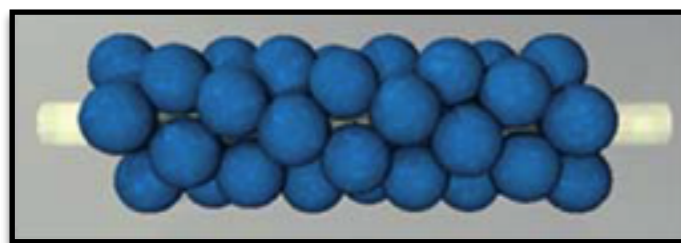
Mughal and Weaire, PRE 89:042307 (2014)



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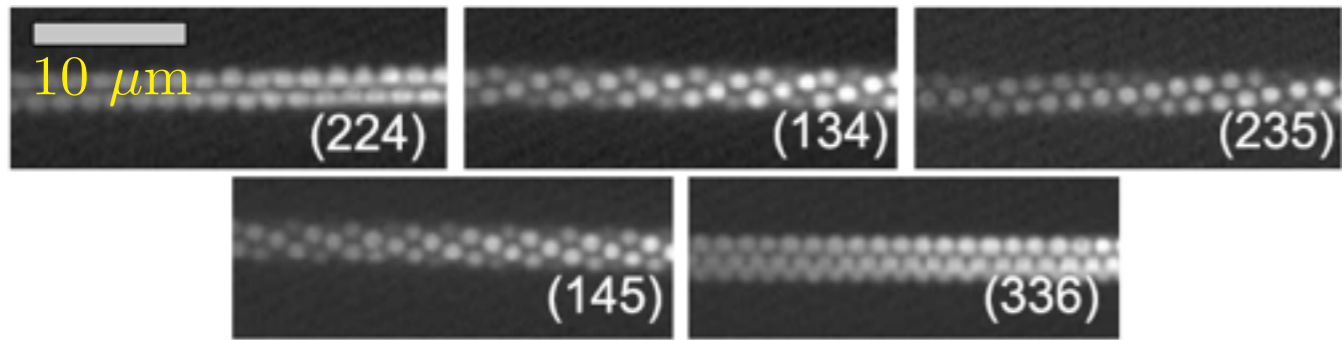


Rhombic lattice favored for soft potentials

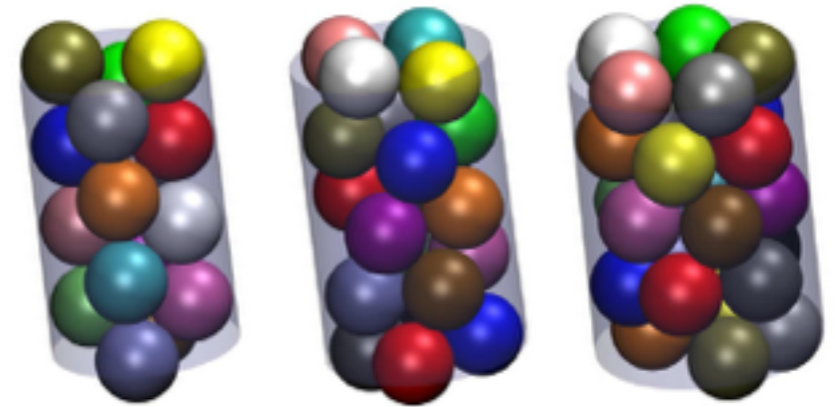
Wood et al., Soft Matter 9:10016 (2013)

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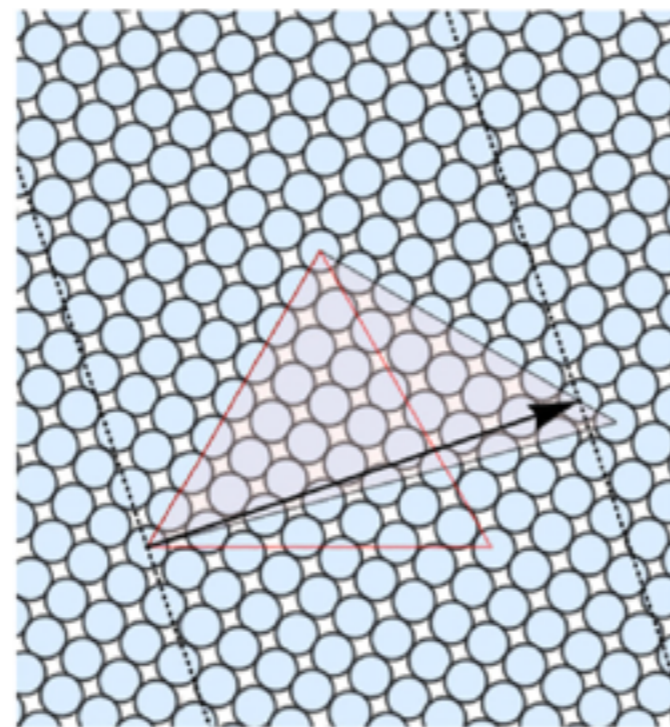
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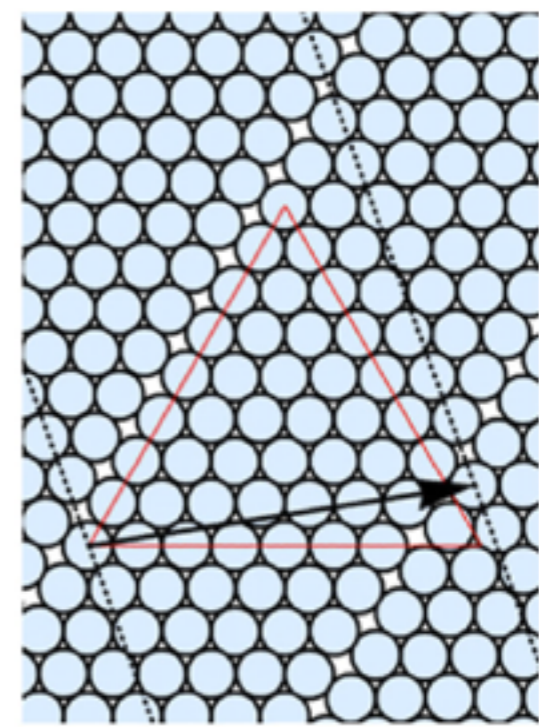
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What happens if the cylinder radius is incommensurate with any perfect phyllotactic packing?

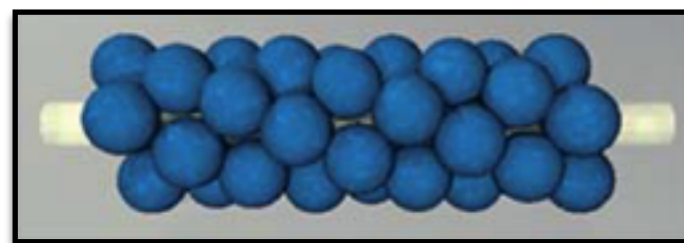
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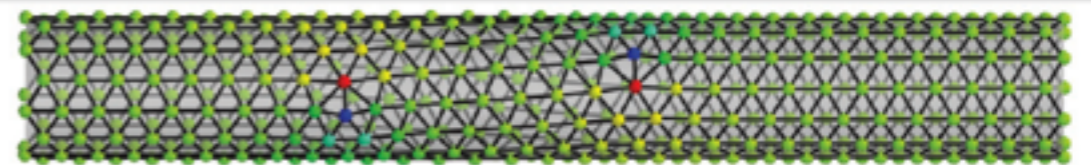


Helical "line-slip" defects in a triangular lattice



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Dislocation interaction energetics on a cylinder

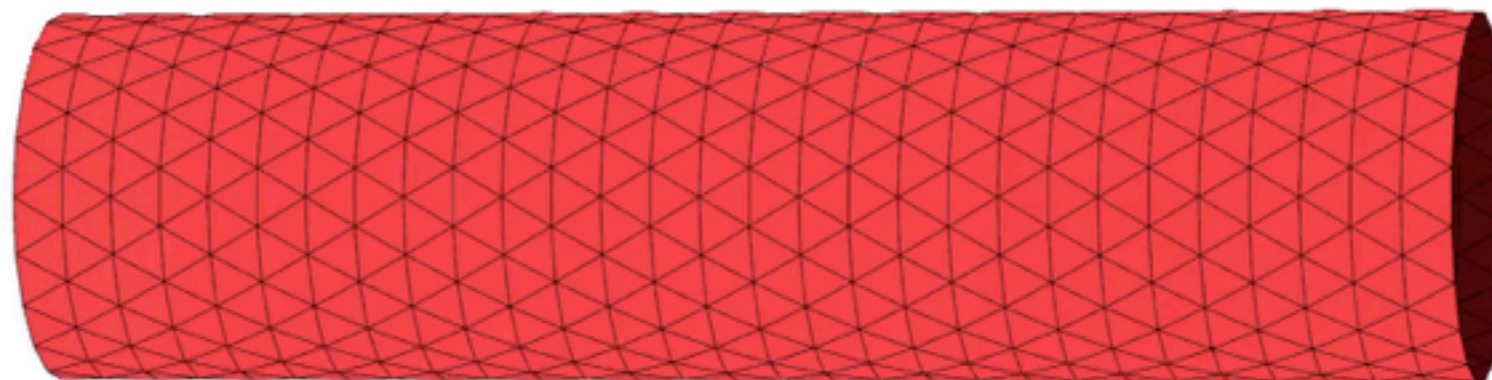
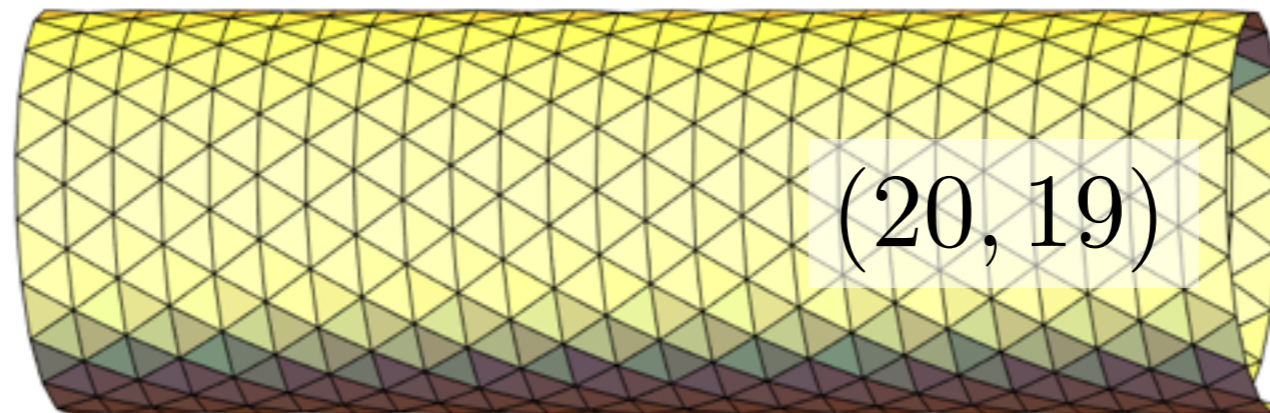
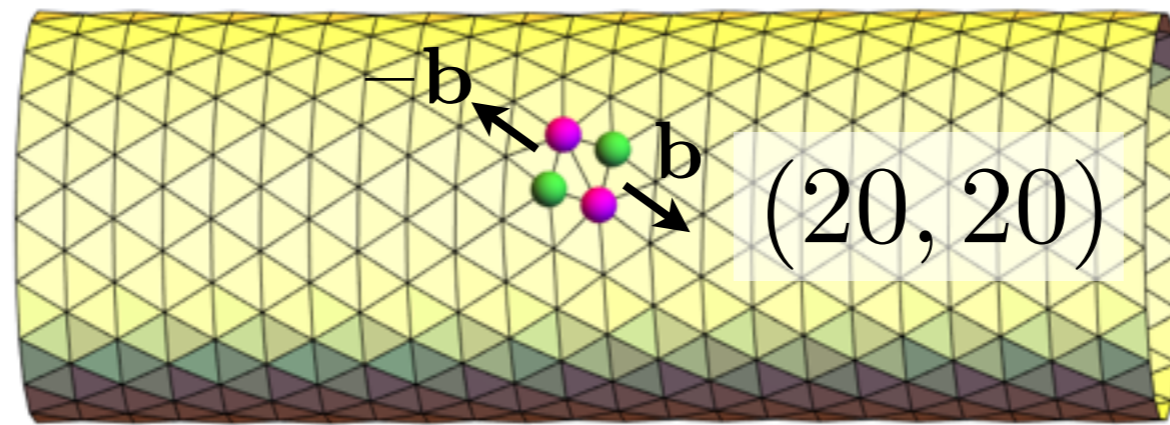


Amir, Paulose, Nelson, PRE 87:042314 (2013)

This work:

Dislocation-mediated plastic deformation of tubular crystals
where the tube radius is *not fixed*:

R varies in space and time

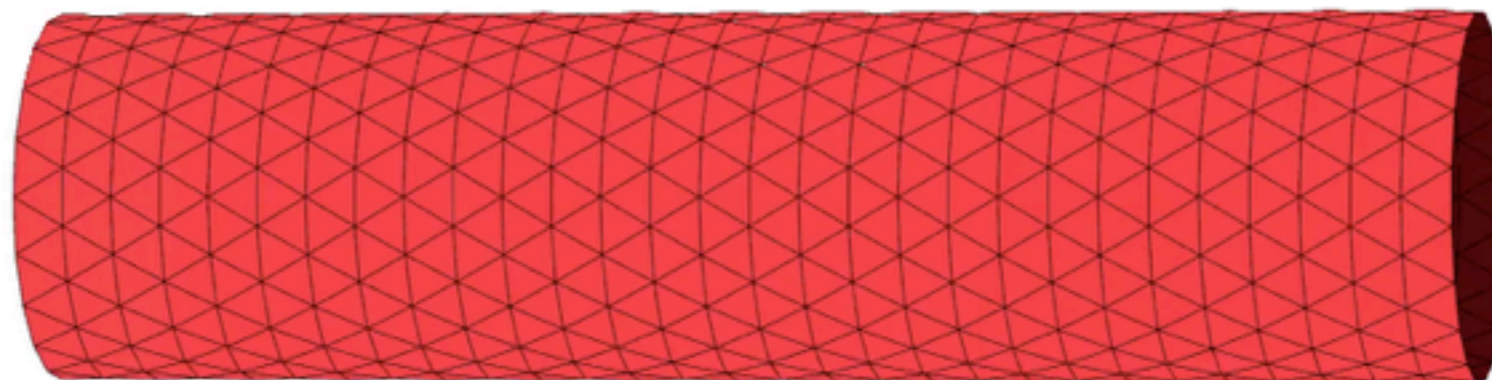
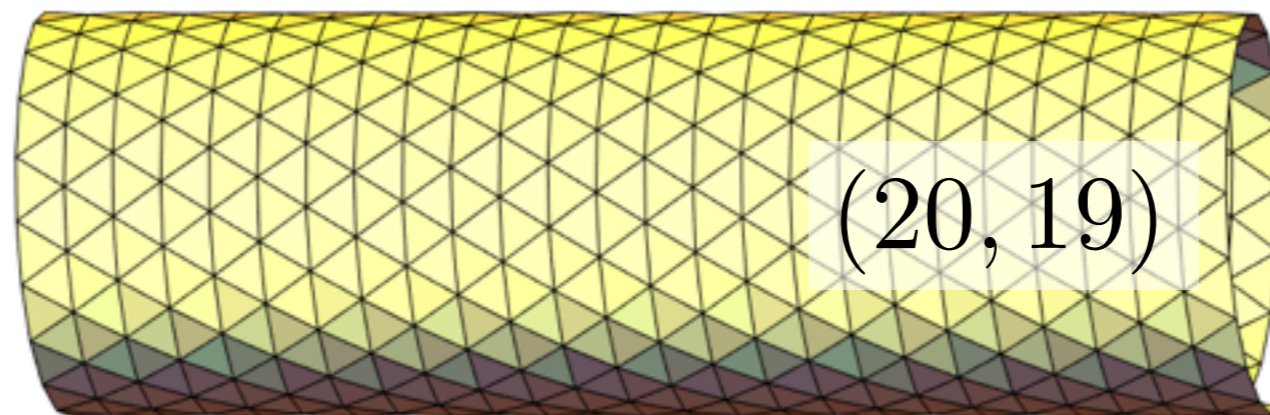
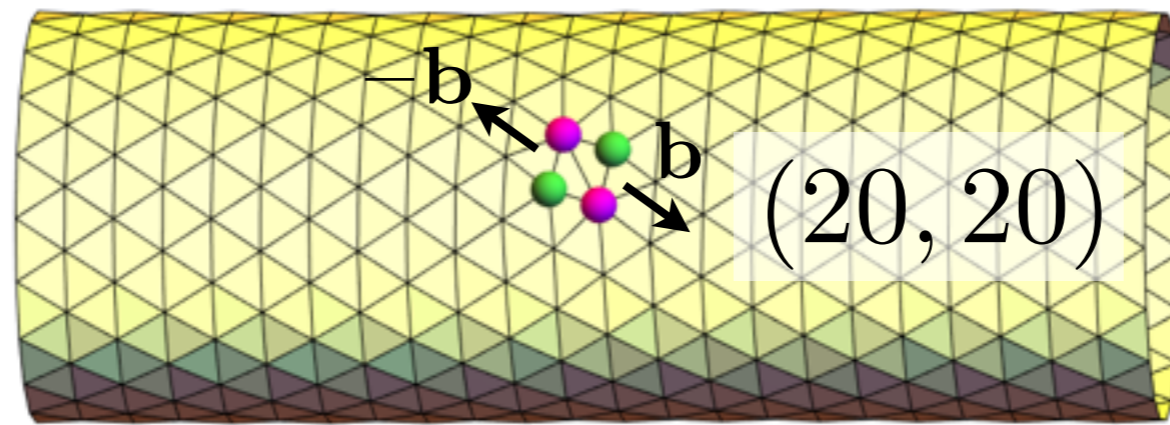


Radius/lattice spacing

This work:

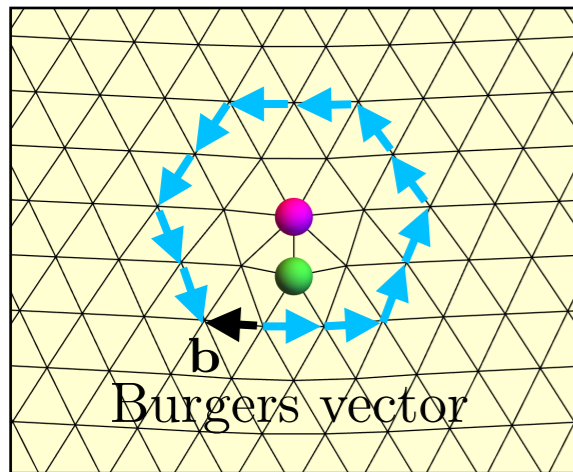
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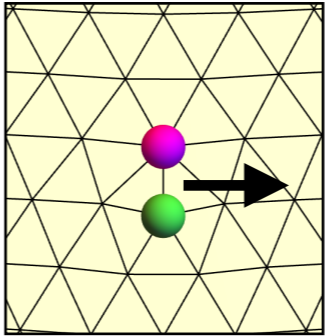


Radius/lattice spacing

Dislocation motion: Glide and climb


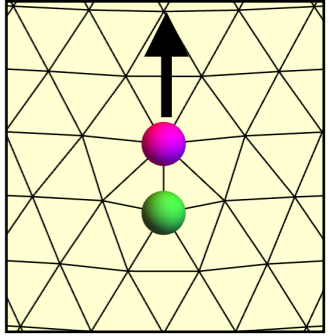


Glide: $dx/dt \parallel \mathbf{b}$

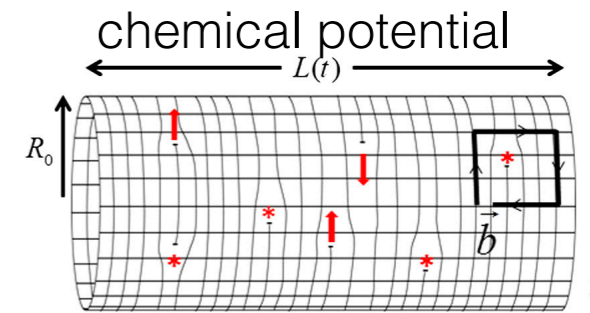



usually easier for mass-conserving systems

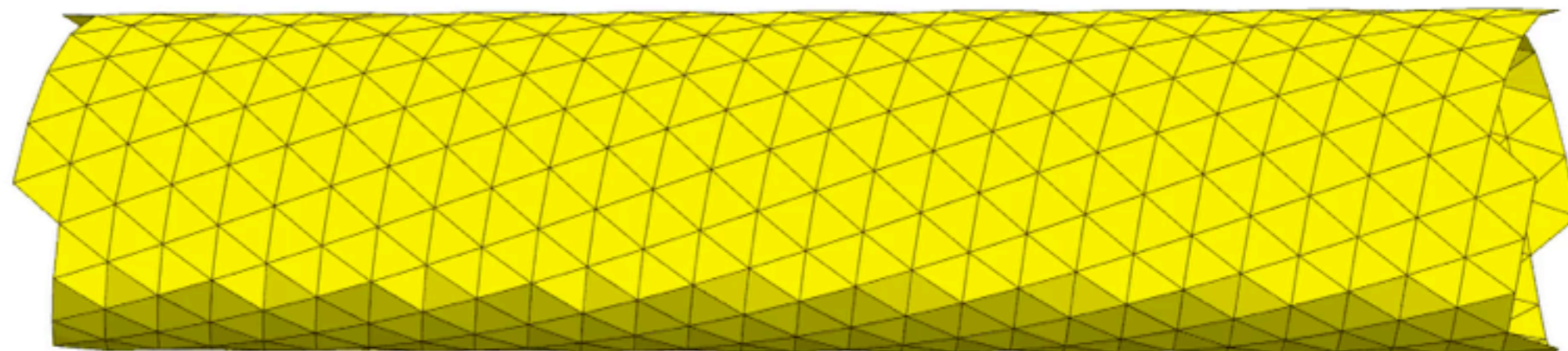
Climb: $dx/dt \perp \mathbf{b}$

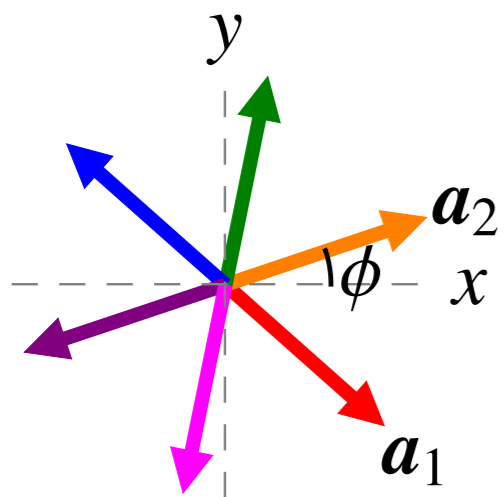
relevant to systems with growth/
chemical potential



e.g., Bacterial cell wall growth
Amir & Nelson, PNAS 109:9833 (2012)

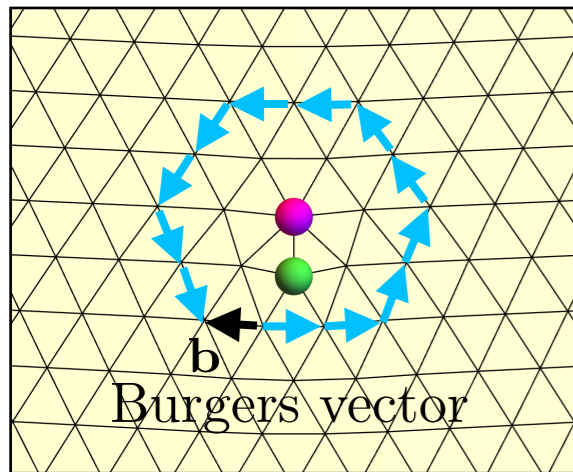


The six elementary Burgers vector pairs
on a triangular lattice


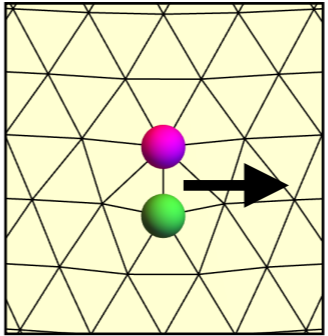


\mathbf{b} of the
right-moving dislocation

Dislocation motion: Glide and climb


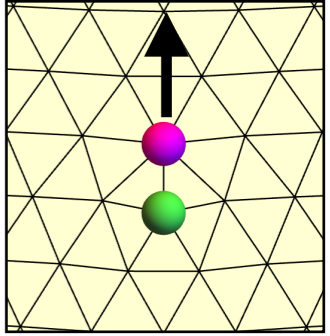


Glide: $dx/dt \parallel \mathbf{b}$

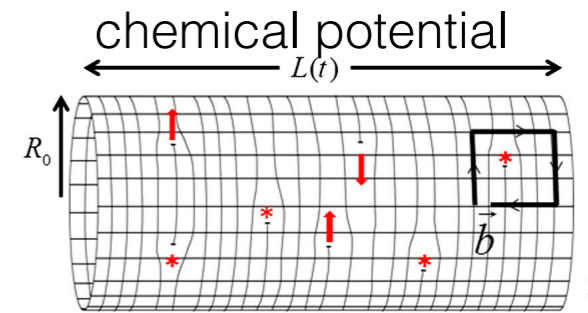



usually easier for mass-conserving systems

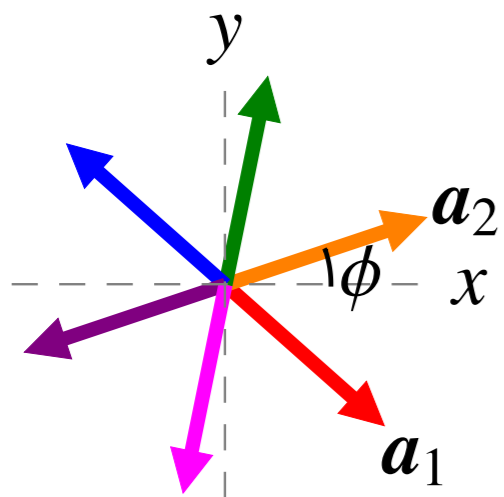
Climb: $dx/dt \perp \mathbf{b}$

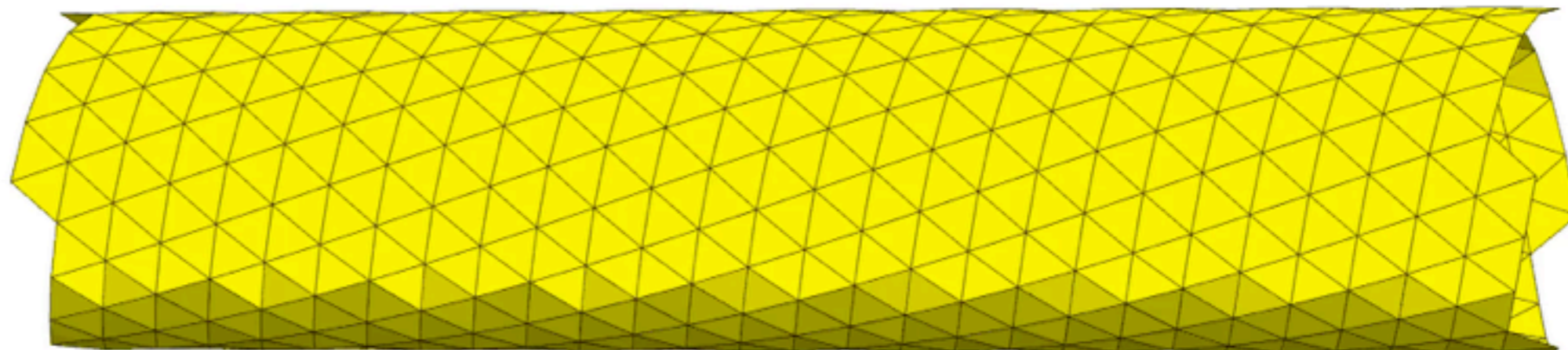
relevant to systems with growth/
chemical potential



e.g., Bacterial cell wall growth
Amir & Nelson, PNAS 109:9833 (2012)



\mathbf{b} of the
right-moving dislocation



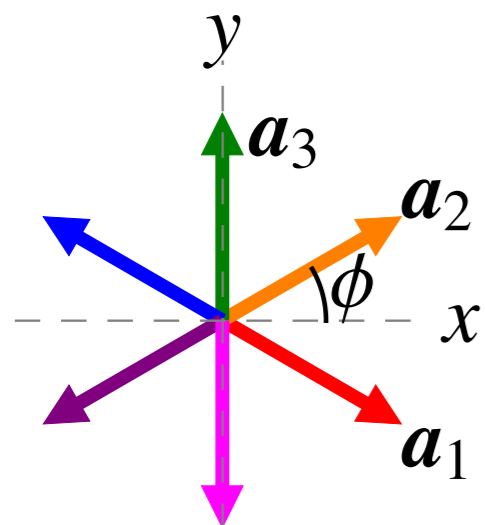
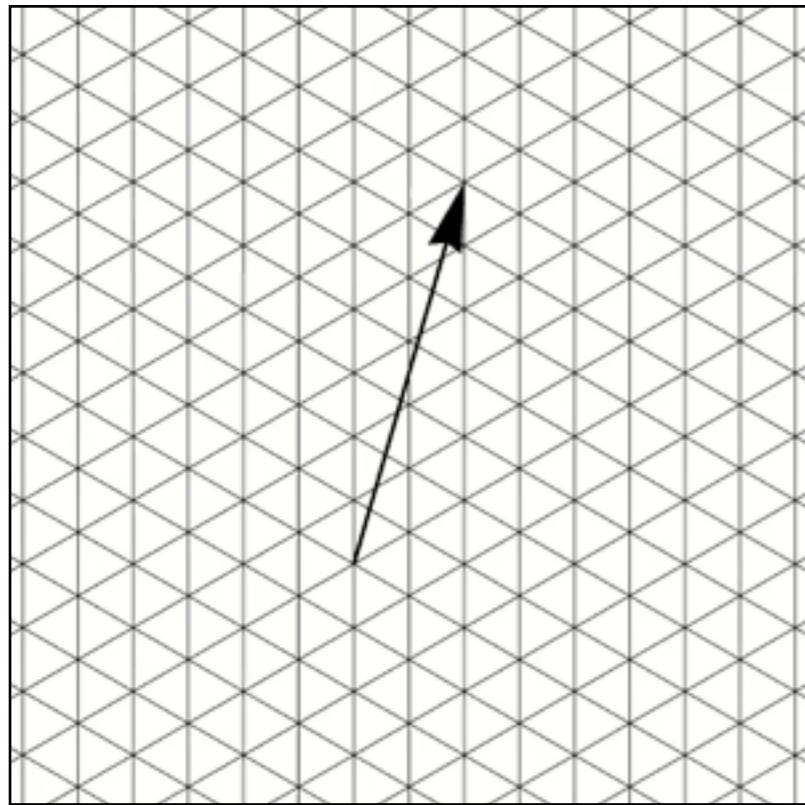
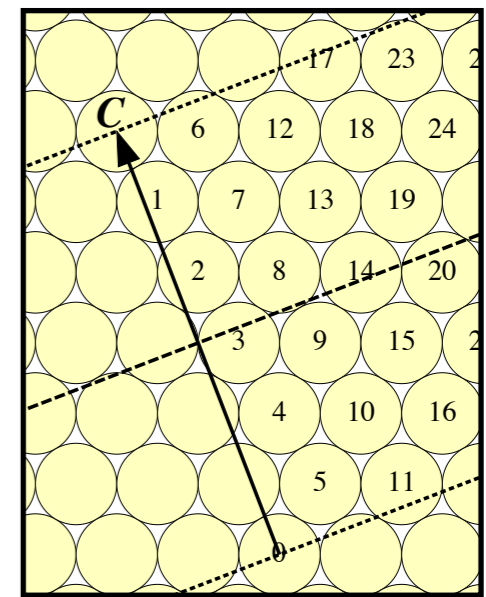
The six elementary Burgers vector pairs
on a triangular lattice

A dislocation passing through the system changes (m, n)

Altered circumference vector:

$$\mathbf{C}' = \mathbf{C} + \mathbf{b}$$

$$\mathbf{C} = m\mathbf{a}_2 - n\mathbf{a}_1$$

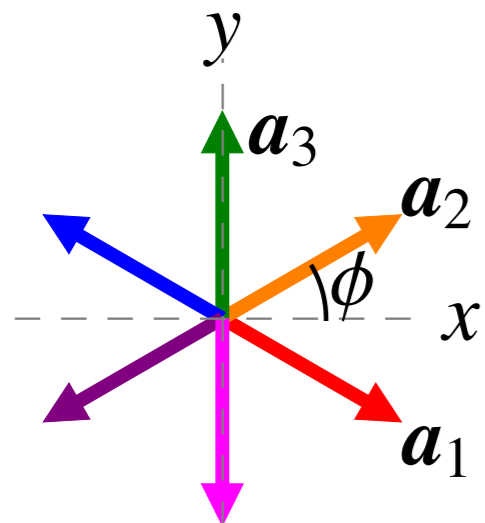
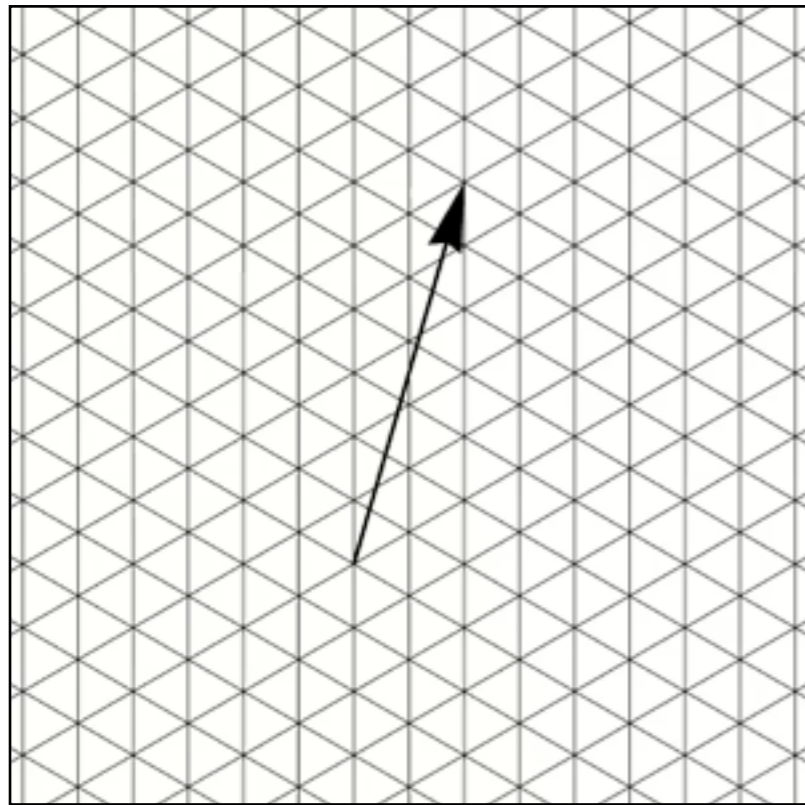
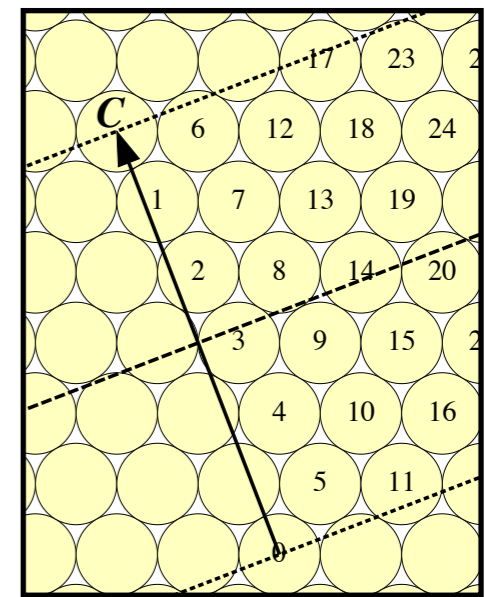


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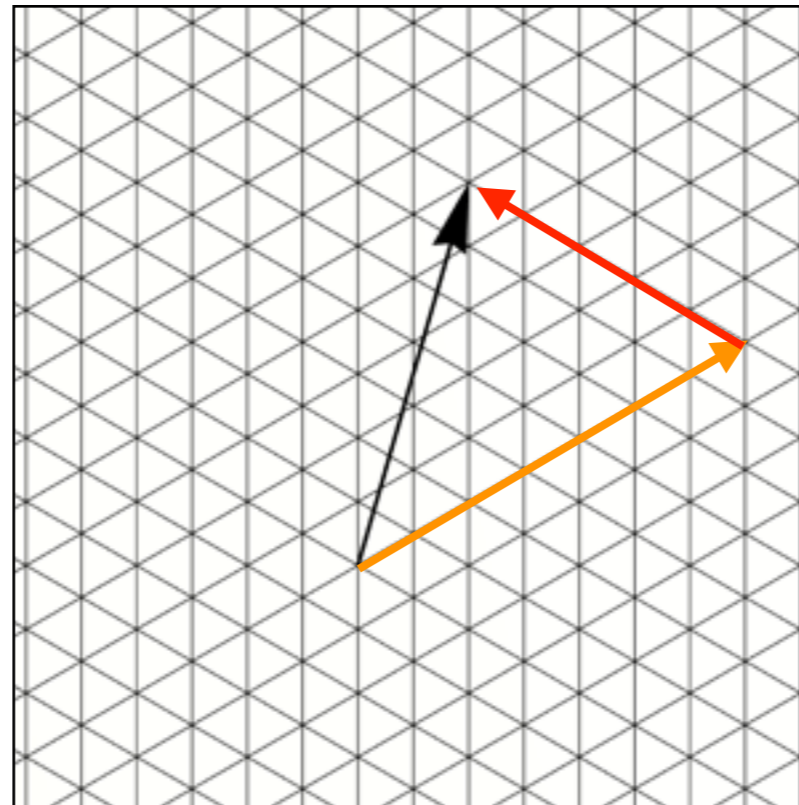
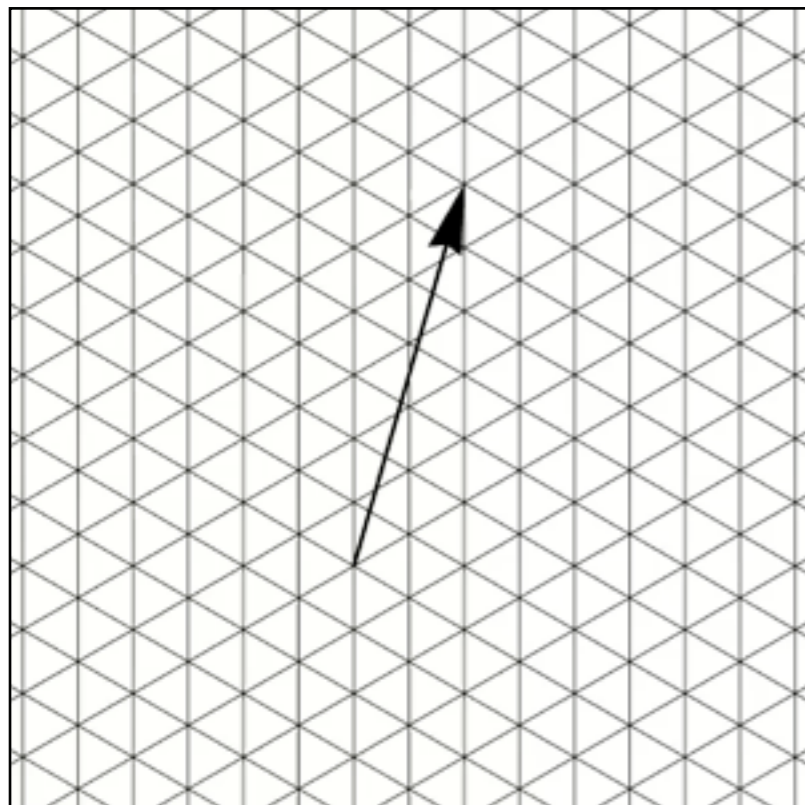
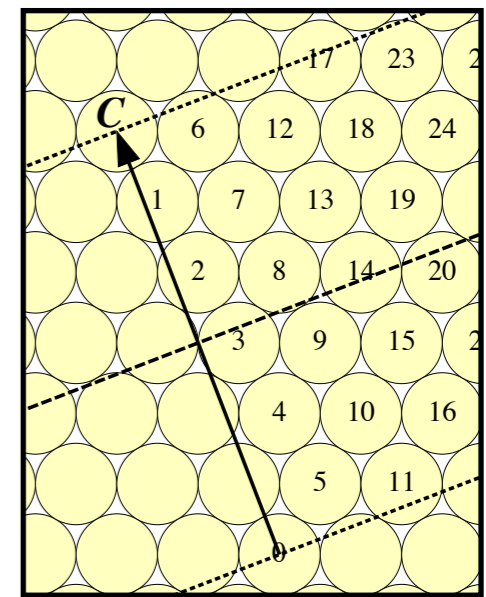


A dislocation passing through the system changes (m, n)

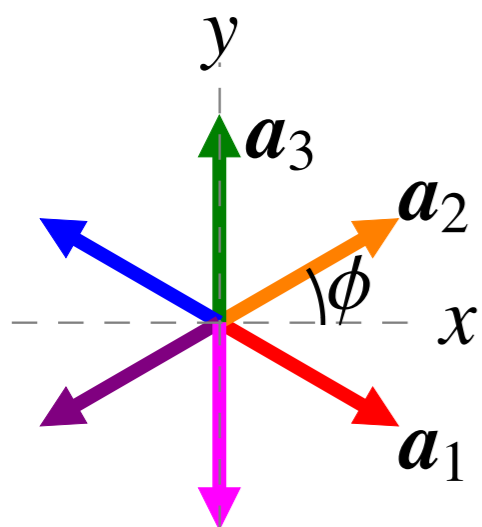
Altered circumference vector:

$$\mathbf{C}' = \mathbf{C} + \mathbf{b}$$

$$\mathbf{C} = m\mathbf{a}_2 - n\mathbf{a}_1$$



$$\mathbf{C} = 7\mathbf{a}_2 - 5\mathbf{a}_1$$

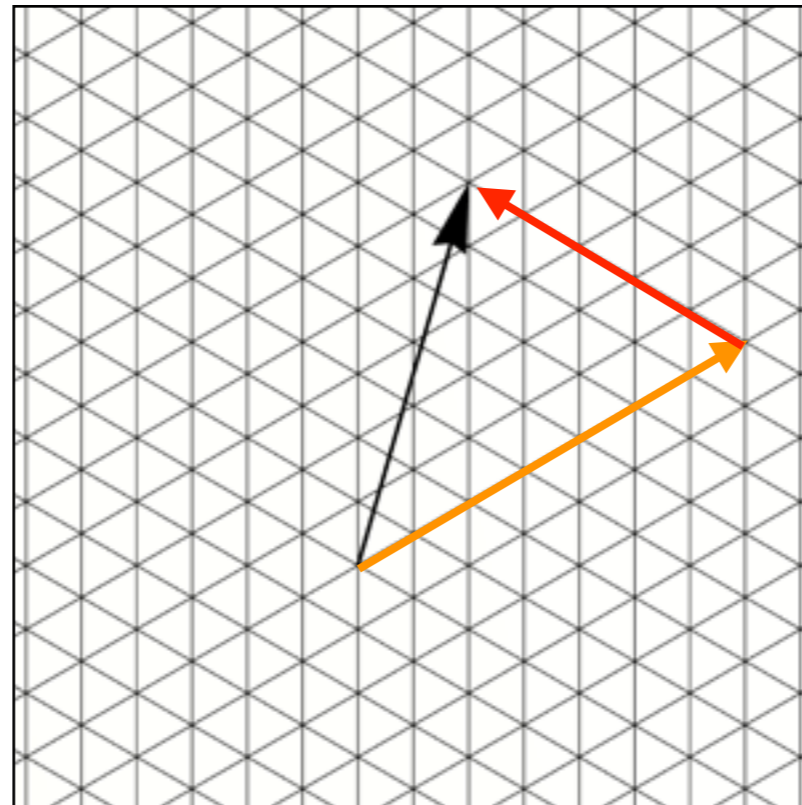
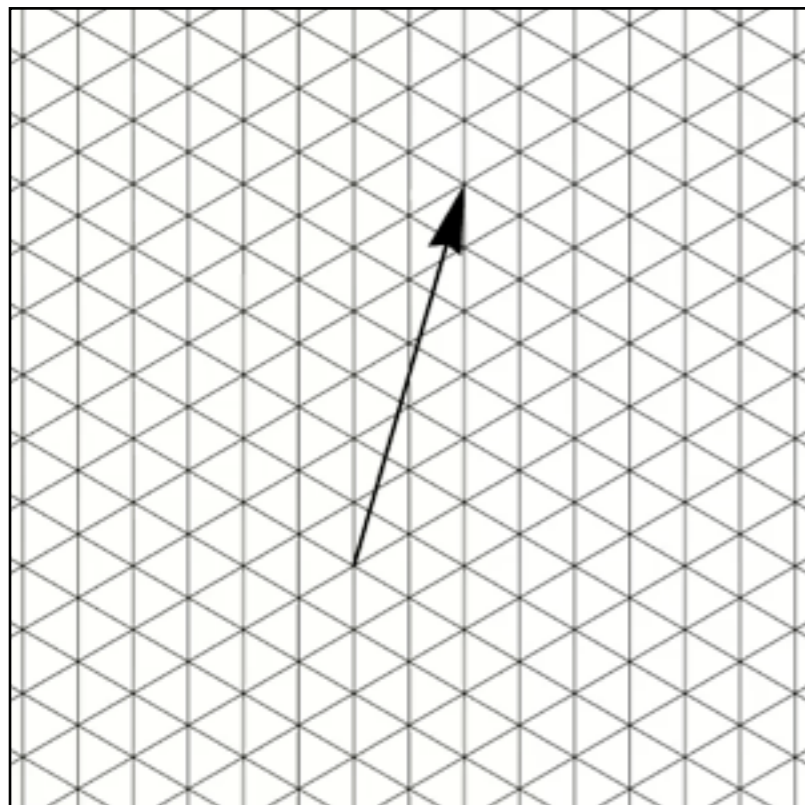
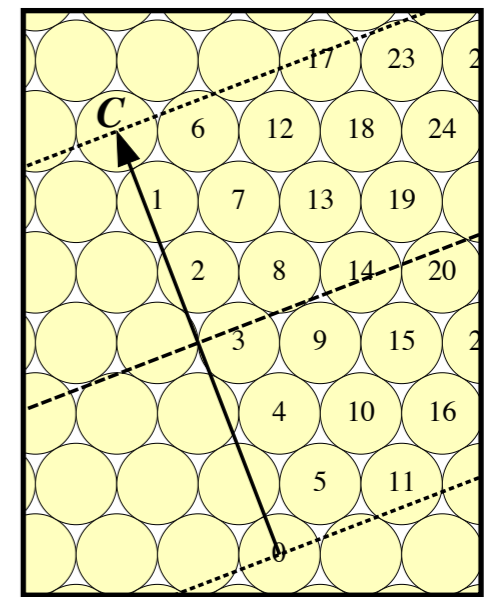


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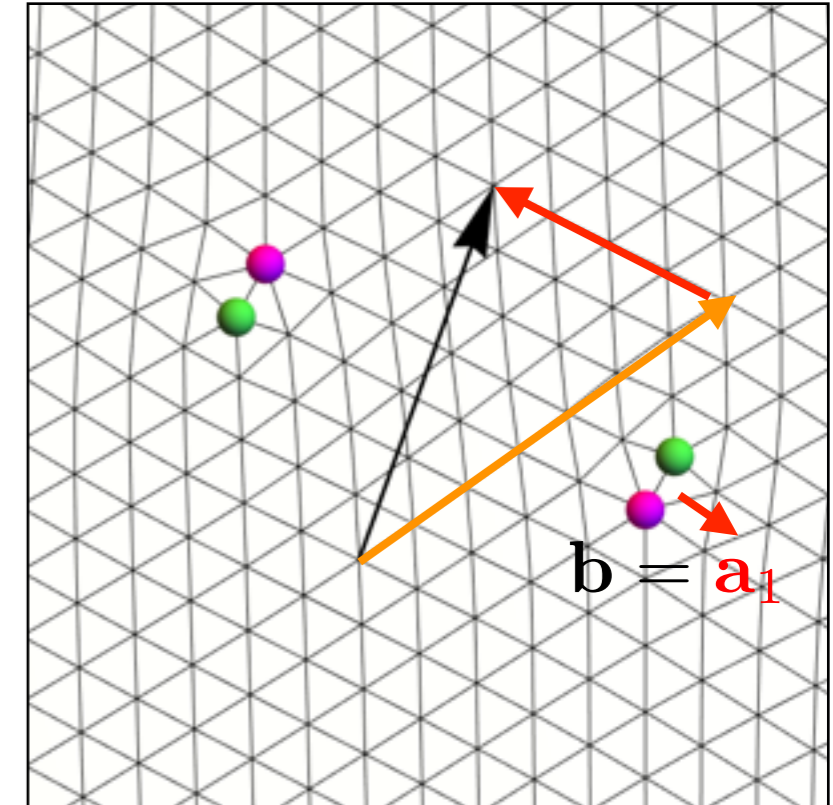
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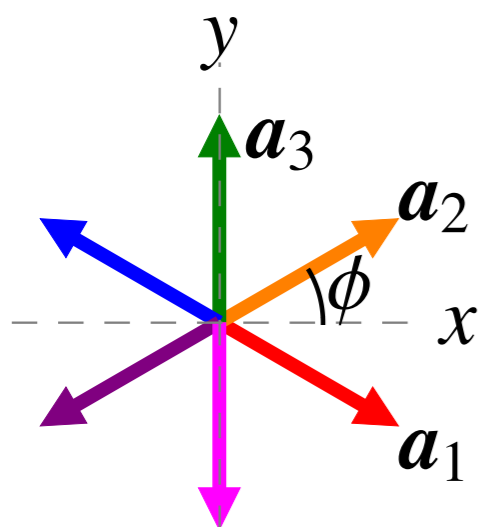


$$\mathbf{C} = 7\mathbf{a}_2 - 5\mathbf{a}_1$$



$$\mathbf{C}' = 7\mathbf{a}_2 - 4\mathbf{a}_1$$

$(m, n) \rightarrow (m, n - 1)$

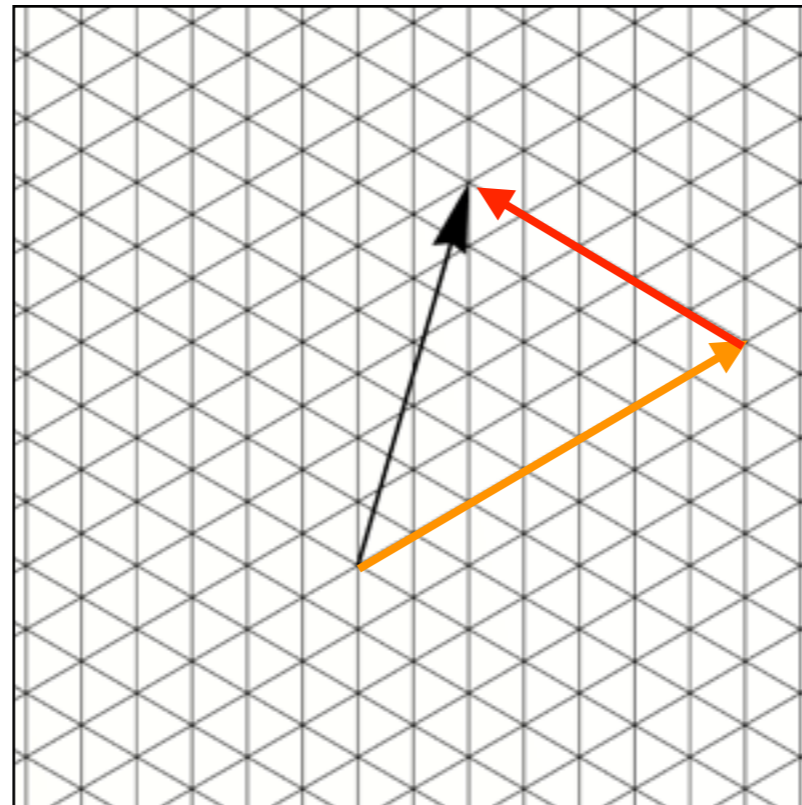
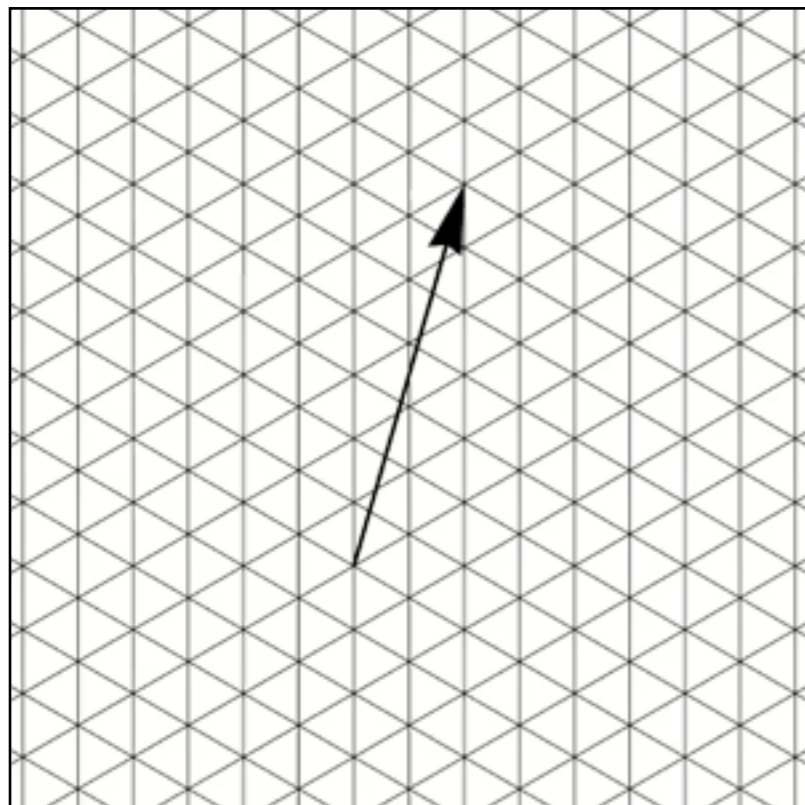
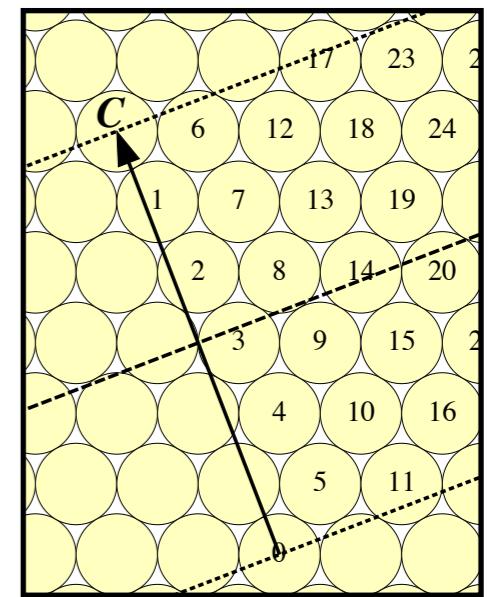


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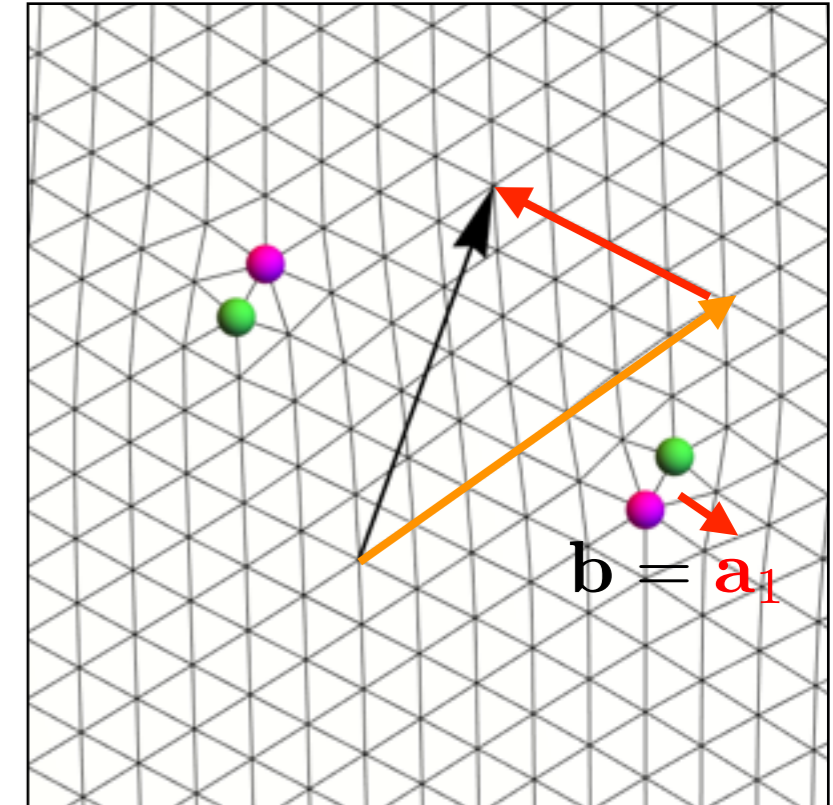
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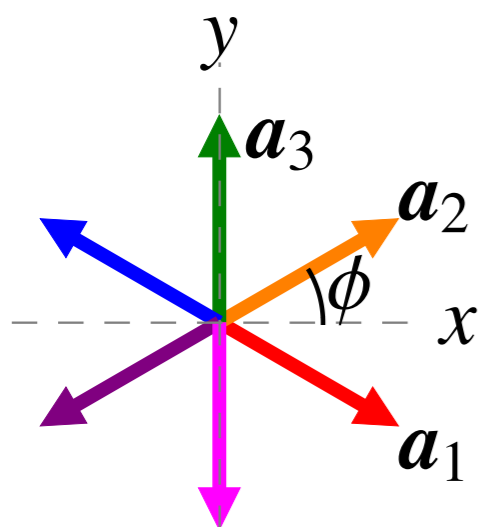


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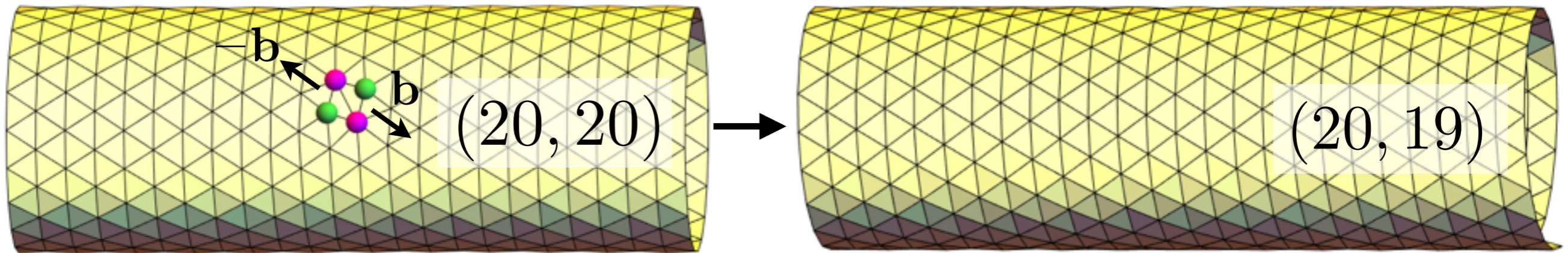
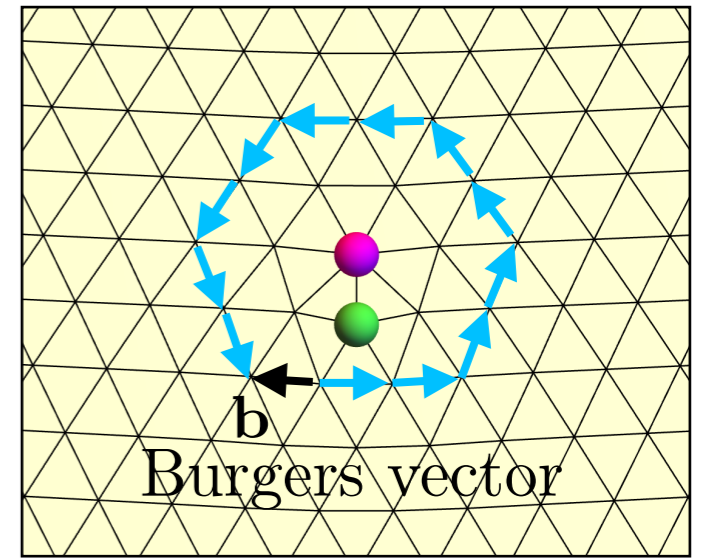
$(m, n) \rightarrow (m, n - 1)$



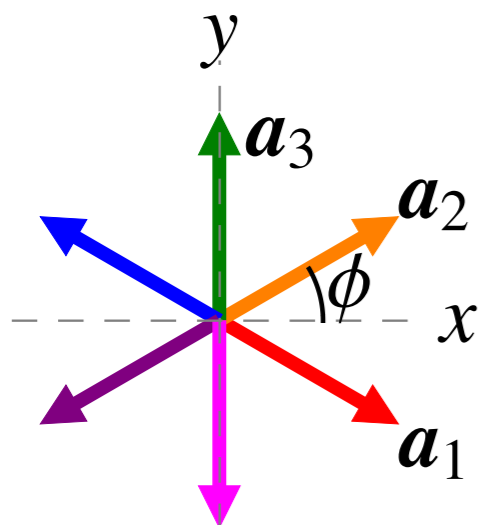
\mathbf{b}	\mathbf{a}_1	\mathbf{a}_2	\mathbf{a}_3	$-\mathbf{a}_1$	$-\mathbf{a}_2$	$-\mathbf{a}_3$
Δm	0	+1	+1	0	-1	-1
Δn	-1	0	+1	+1	0	-1

A dislocation passing through the system changes (m,n)

Altered circumference vector: $\mathbf{C}' = \mathbf{C} + \mathbf{b}$



The right-moving dislocation has $\mathbf{b} = \mathbf{a}_1$

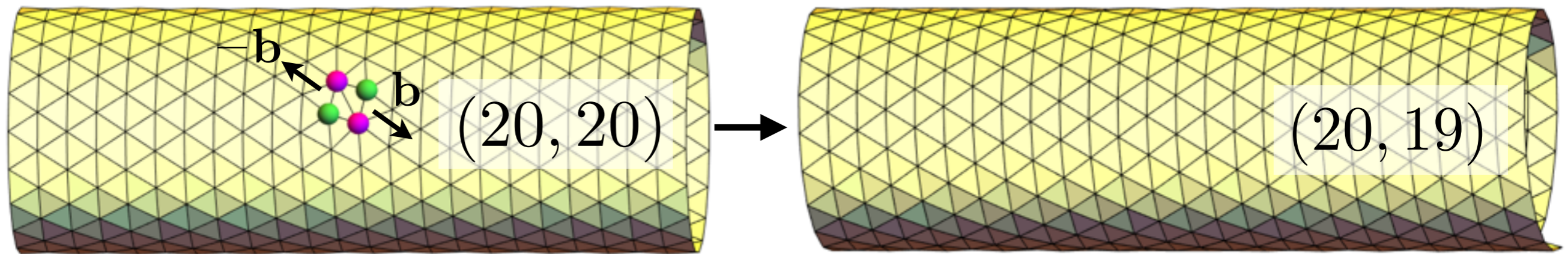
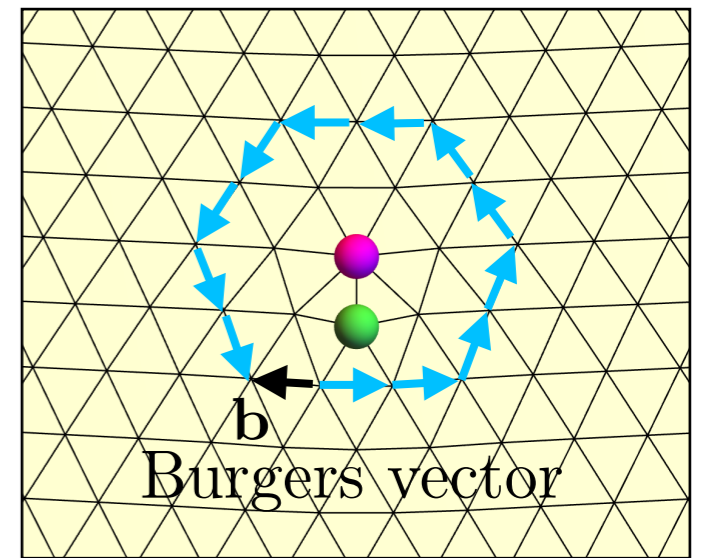


\mathbf{b}	\mathbf{a}_1	\mathbf{a}_2	\mathbf{a}_3	$-\mathbf{a}_1$	$-\mathbf{a}_2$	$-\mathbf{a}_3$
Δm	0	+1	+1	0	-1	-1
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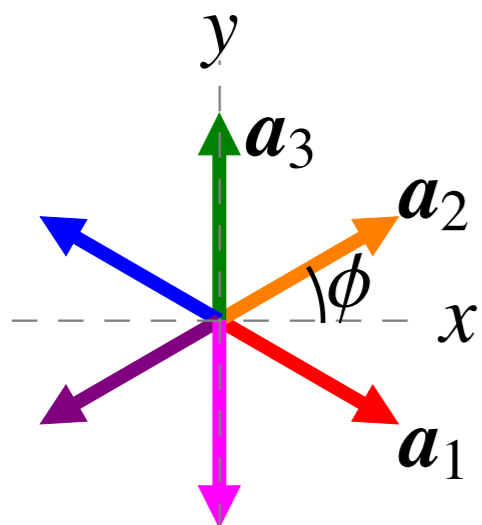
Altered circumference vector:

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The right-moving dislocation has $\mathbf{b} = \mathbf{a}_1$

Dislocation motion \Rightarrow Parastichy transition!
 $(\Delta m, \Delta n) \Rightarrow \Delta R, \Delta \phi \Rightarrow$ Plastic deformation!



\mathbf{b}	\mathbf{a}_1	\mathbf{a}_2	\mathbf{a}_3	$-\mathbf{a}_1$	$-\mathbf{a}_2$	$-\mathbf{a}_3$
Δm	0	+1	+1	0	-1	-1
Δn	-1	0	+1	+1	0	-1

Plastic deformation of tubular crystals

- Background: Phyllotactic geometry of tubular crystals
- Mechanics of plastic deformation: Analytic predictions
- Numerical modeling
- Necks in tubes: Radius profiles near dislocations

Energetics of dislocations on the plane

Stretching energy

$$\begin{aligned} E_s &= \frac{1}{2} \int d\mathbf{x} (2\mu u_{ij}u_{ij} + \lambda u_{kk}^2) \\ &= \frac{1}{2} \cdot \frac{3}{8} Y \int d\mathbf{x} (2u_{ij}u_{ij} + u_{kk}^2) \end{aligned}$$

- $\mu, \lambda =$ Lamé coefficients
- “Harmonic springs” assumption:

$$\mu = \lambda = \frac{3}{8} Y$$

where $Y = 4\pi A =$ Young's modulus

- strain tensor $u_{ij} = \frac{1}{2} (\partial_i u_j + \partial_j u_i)$
where $\vec{u}(\mathbf{x}) =$ displacement field

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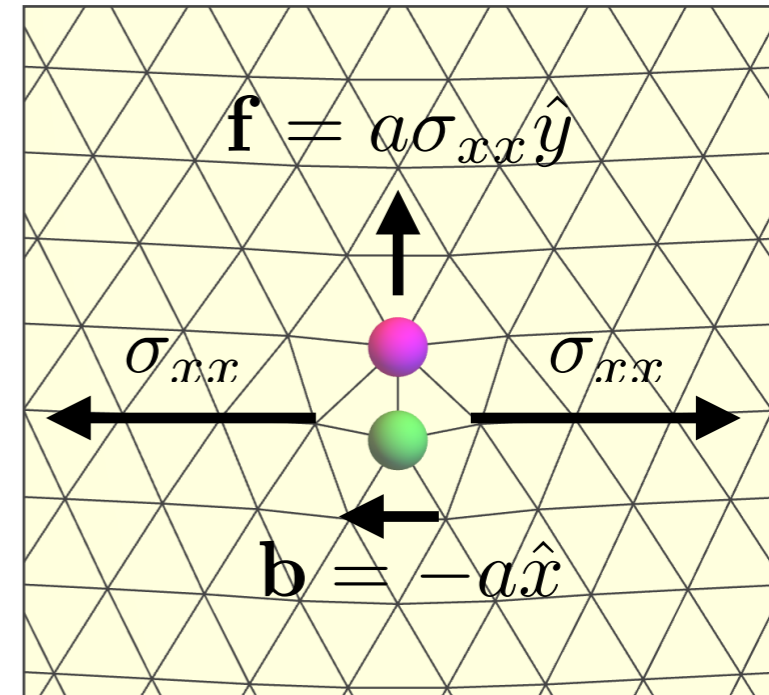
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Peach-Kohler force:
Force on a dislocation \mathbf{b} in a stress field σ

$$f_i = \epsilon_{ijz} b_k \sigma_{jk}$$



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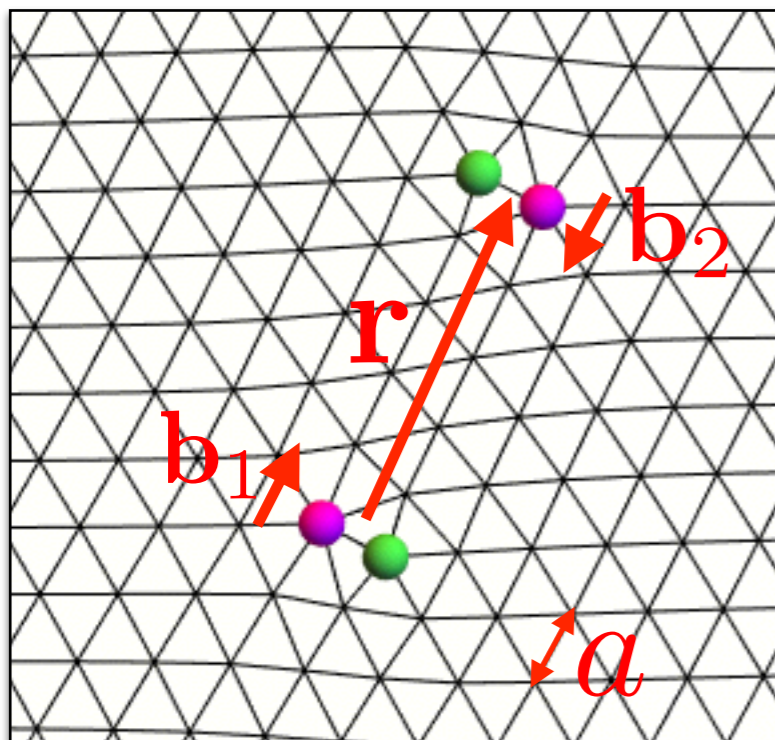
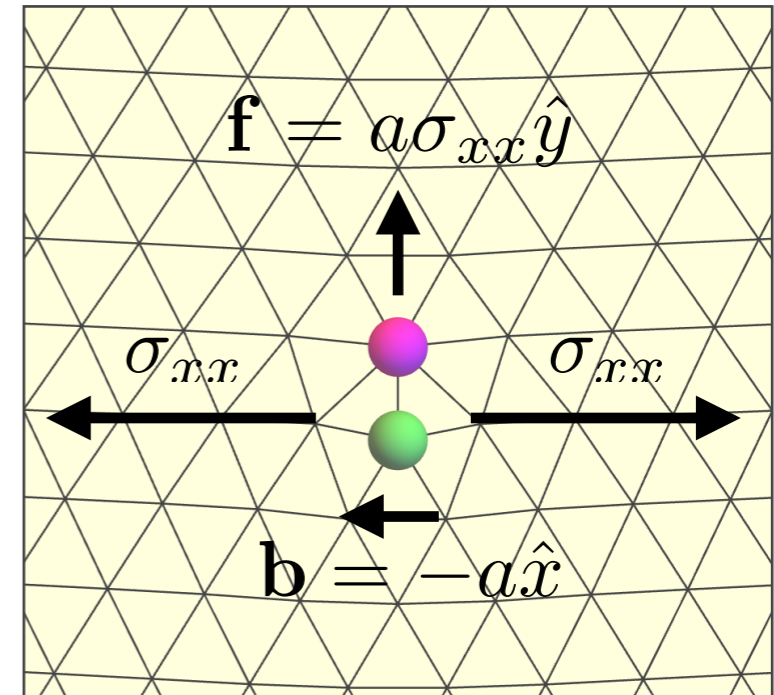
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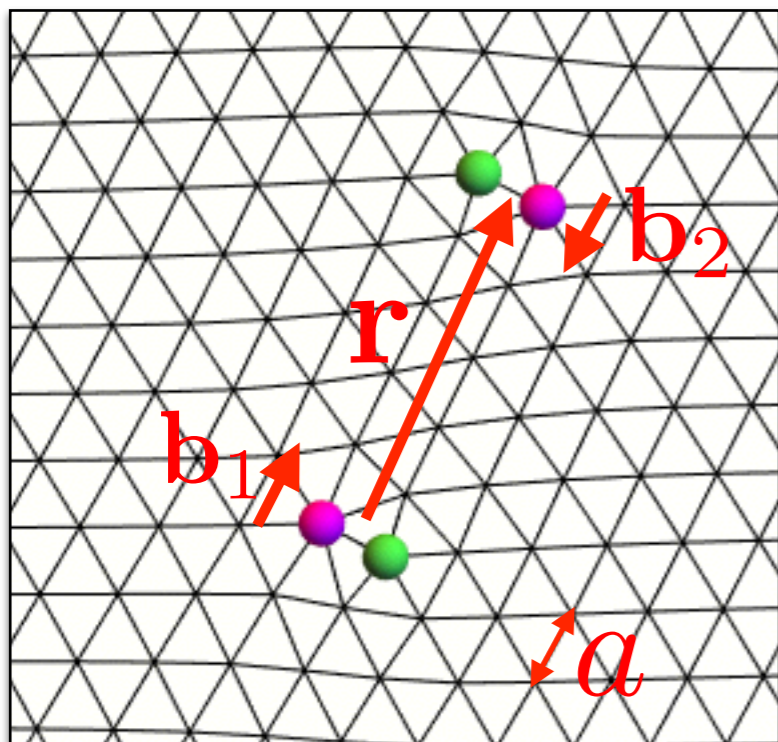
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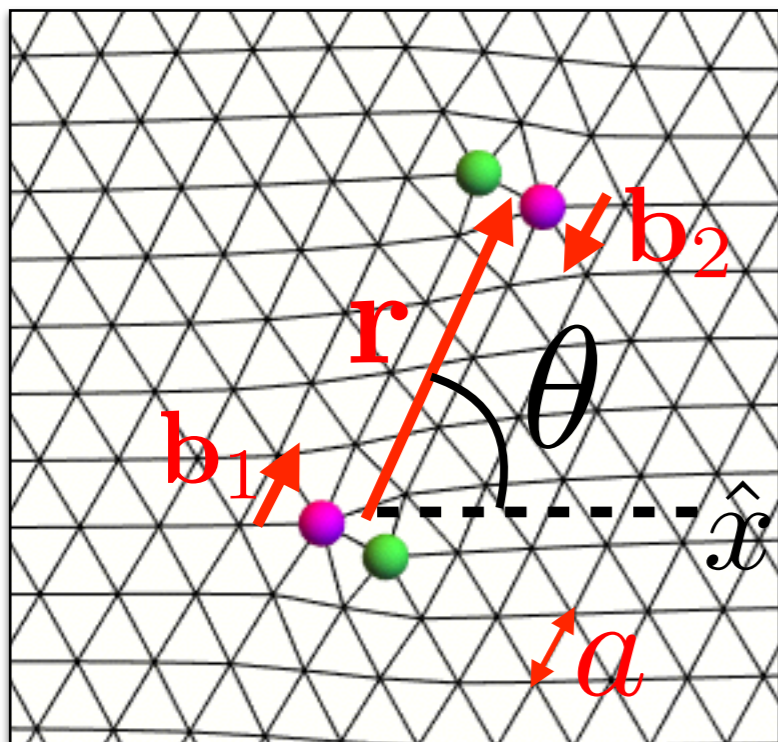
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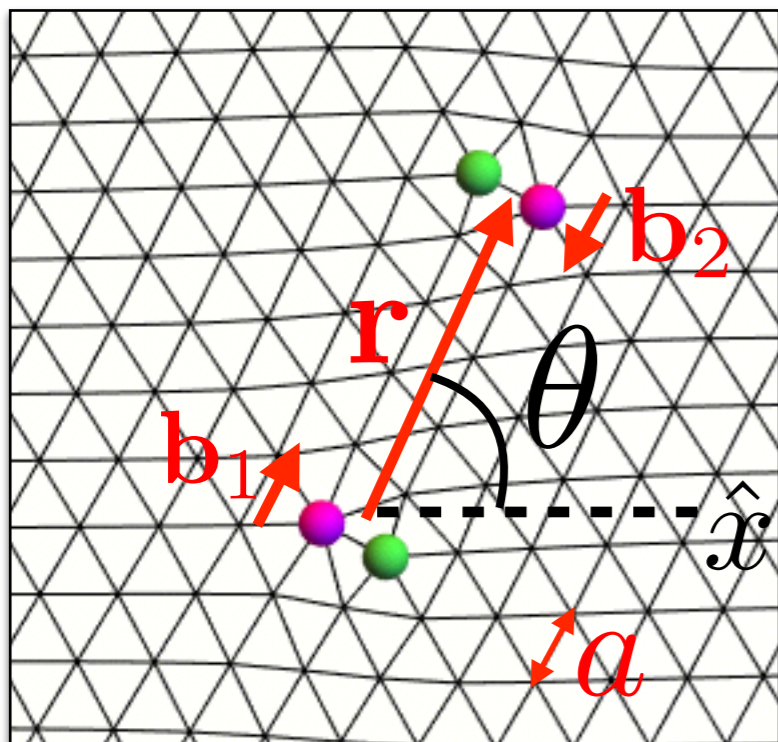
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$$s = \text{sign}[\cos(\theta)]$$

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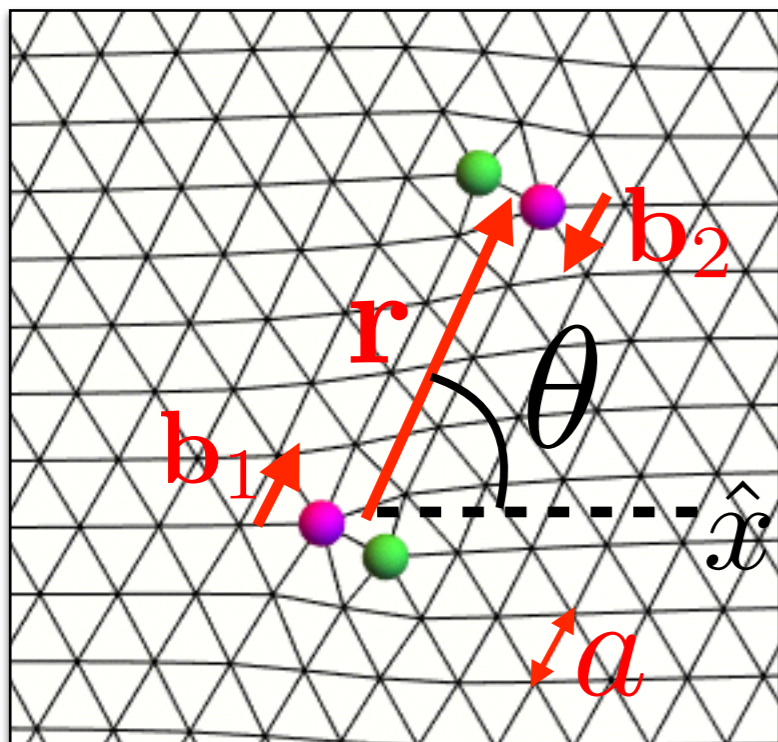
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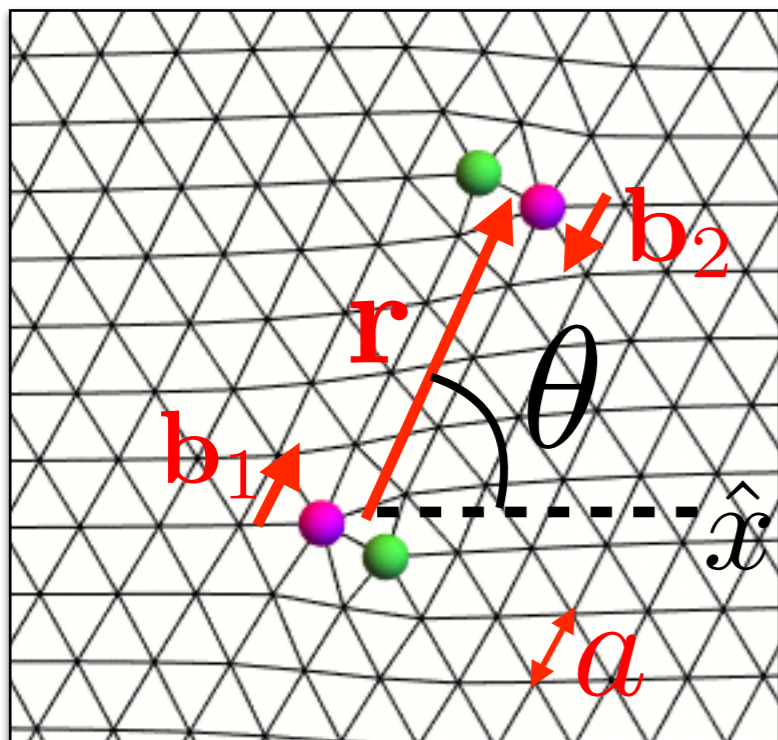
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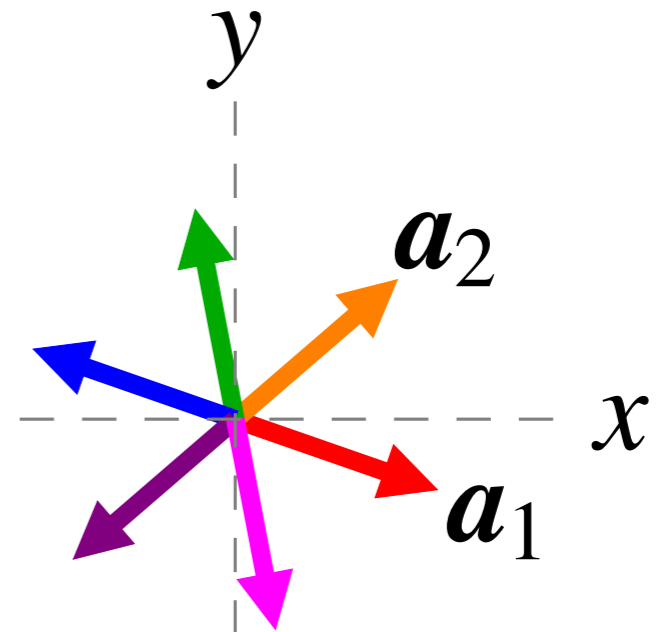
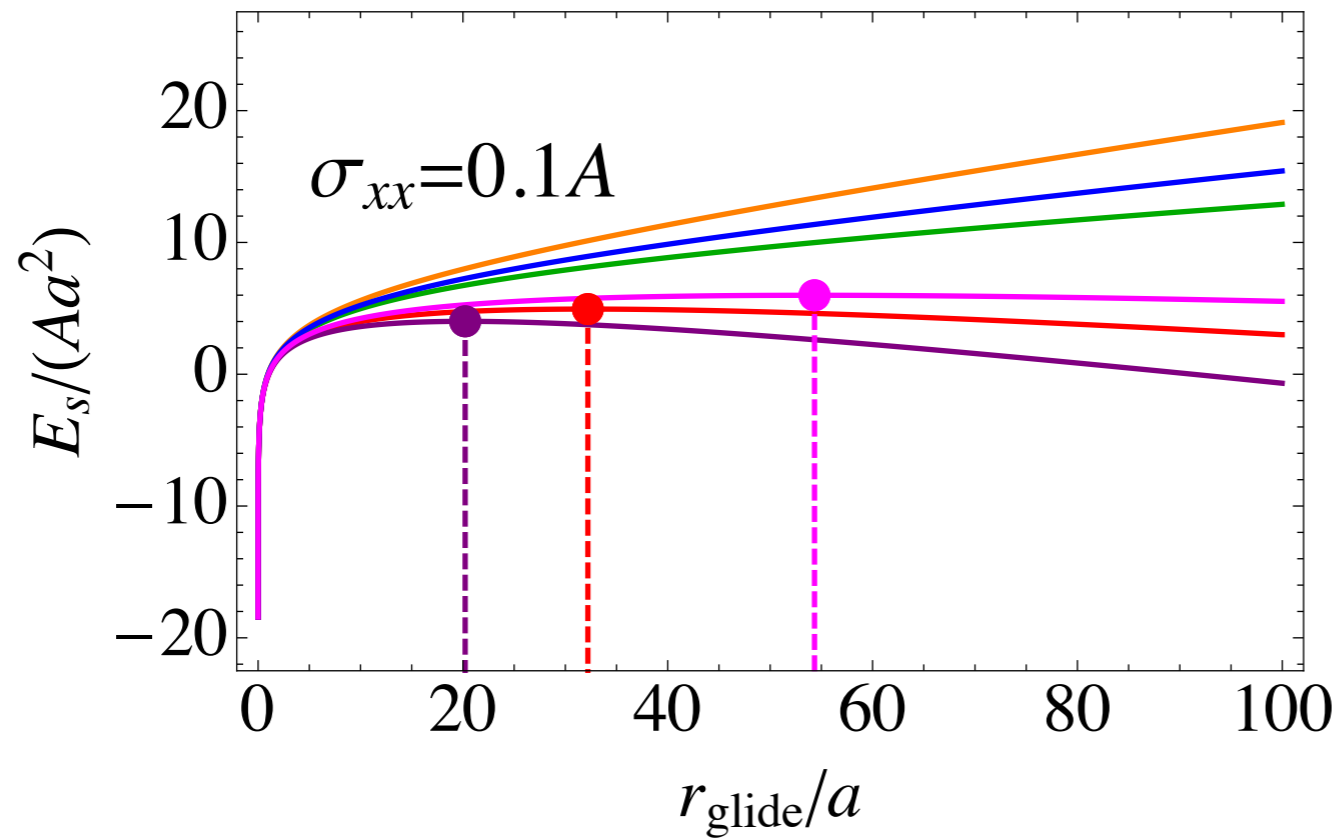
coupling to external stress

$$s = \text{sign}[\cos(\theta)]$$

Dislocation pair energy landscape

$$E_s(r) = Aa^2 \ln(r/a) + s \cdot a \cdot r \cdot \left[\frac{1}{2} \sin(2\theta) (\sigma_{xx}^{\text{ext}} - \sigma_{yy}^{\text{ext}}) - \cos(2\theta) \sigma_{xy}^{\text{ext}} \right] + \text{const.}$$

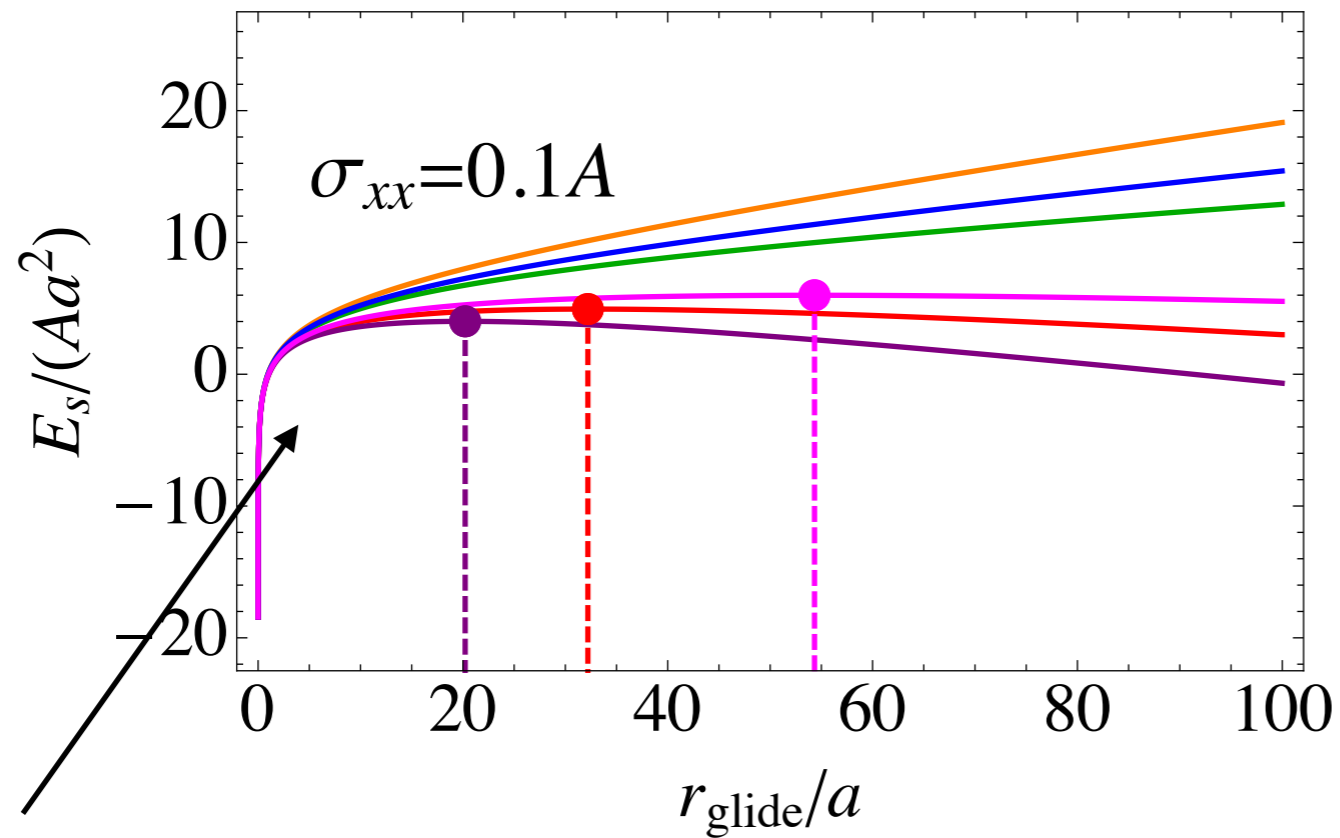
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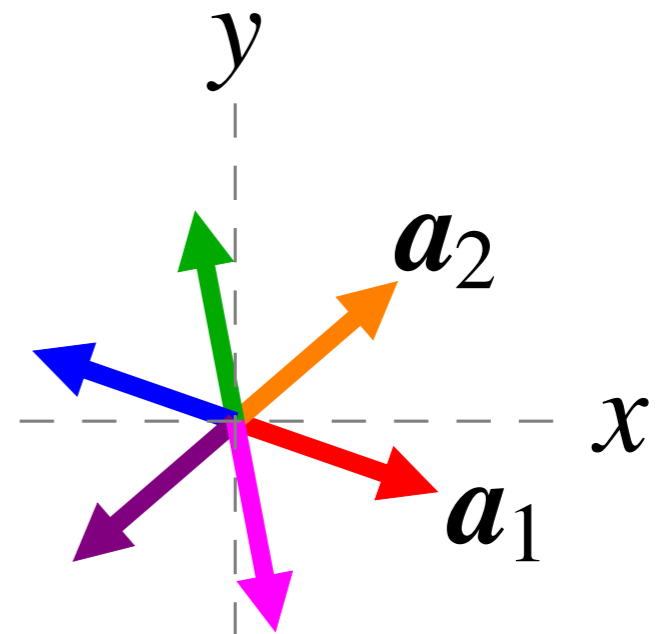
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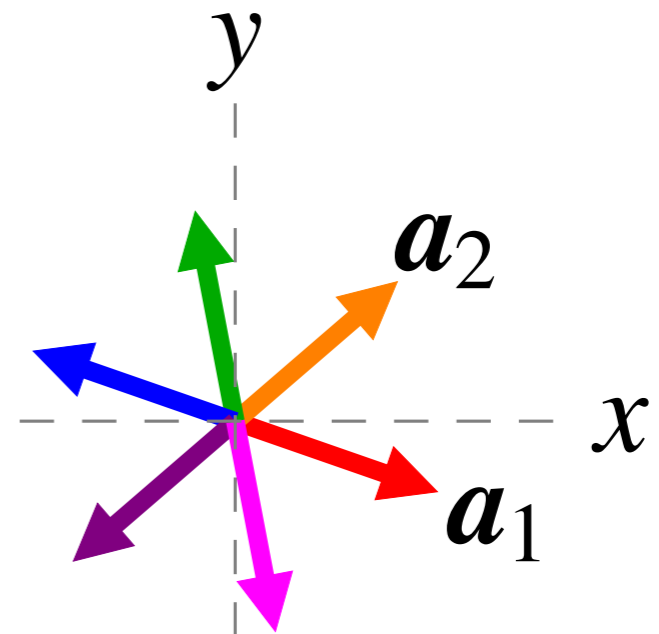
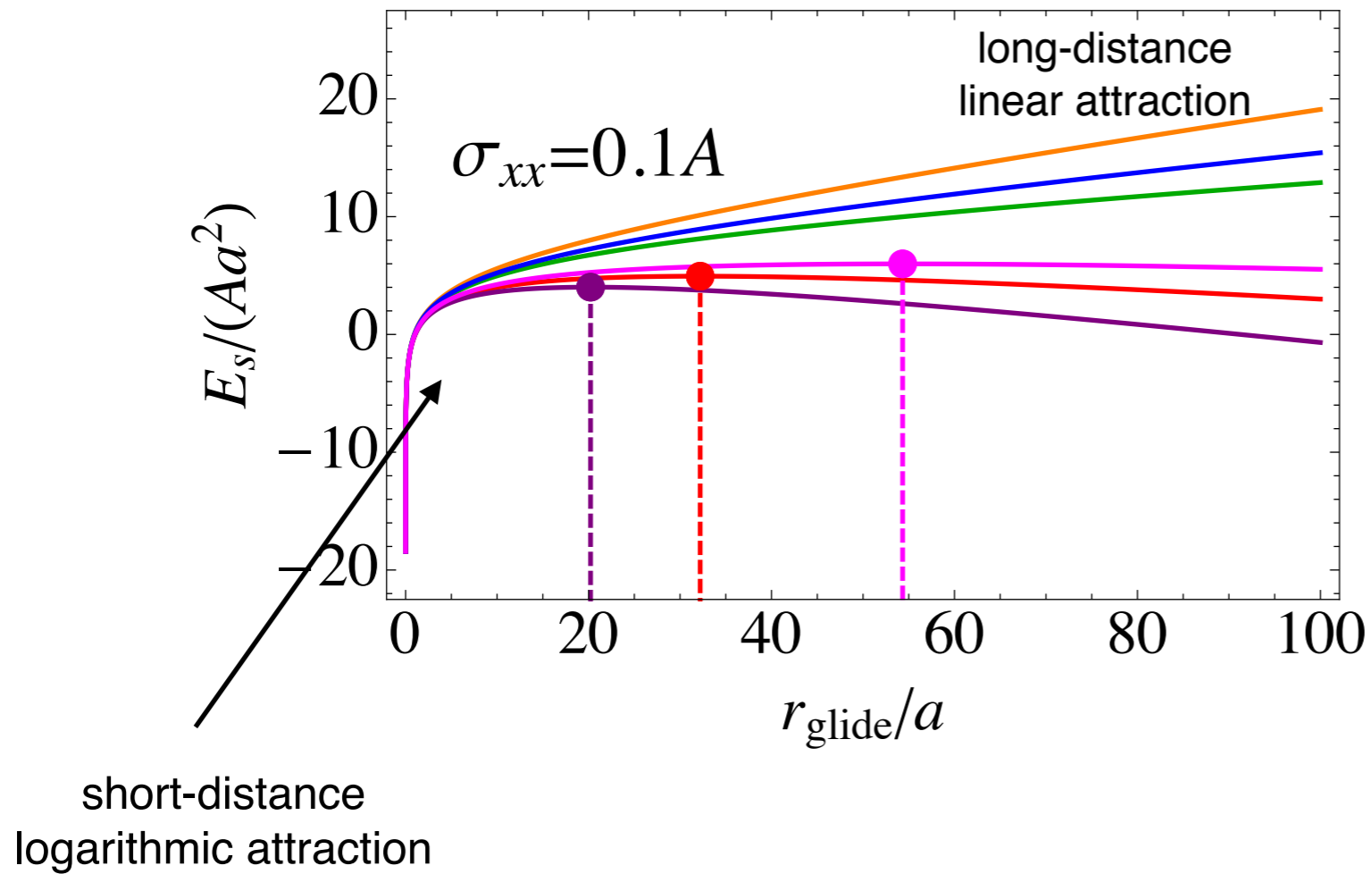
short-distance
logarithmic attraction



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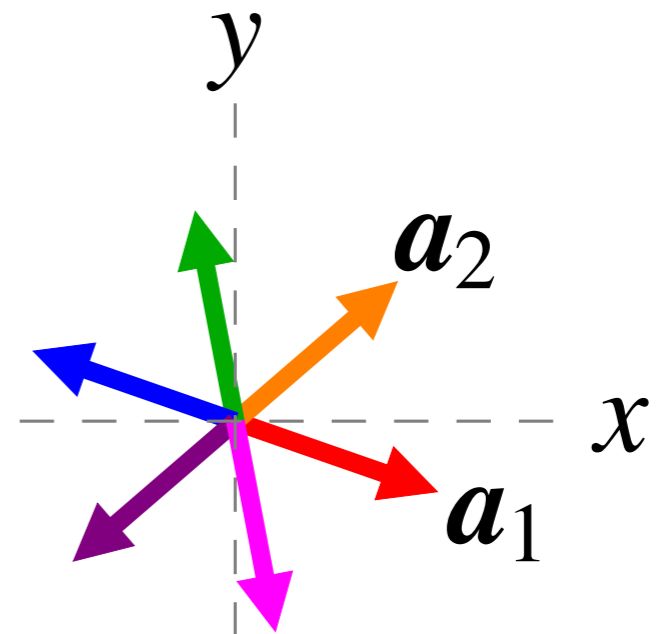
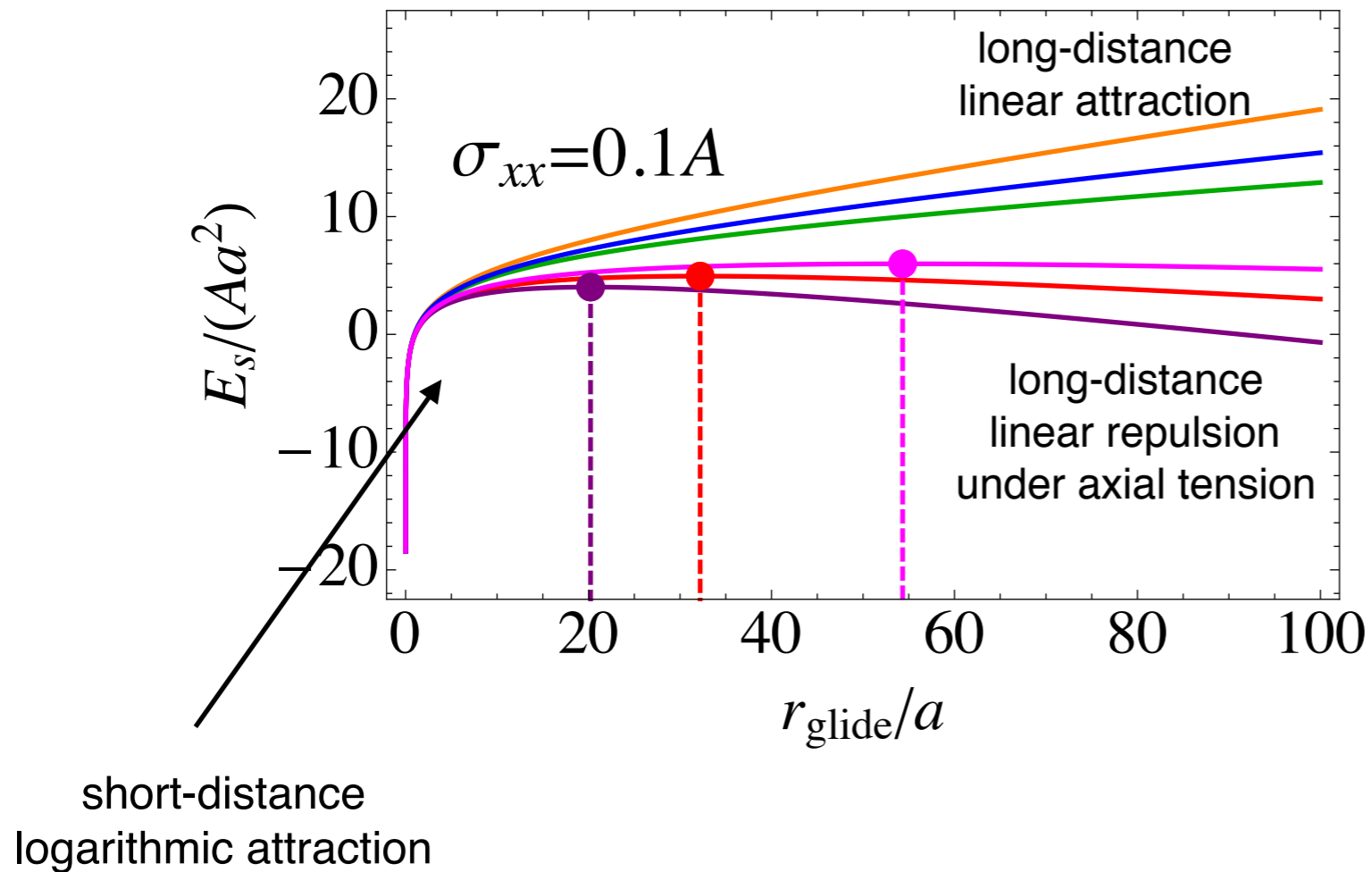
$$s = \text{sign}[\cos(\theta)]$$



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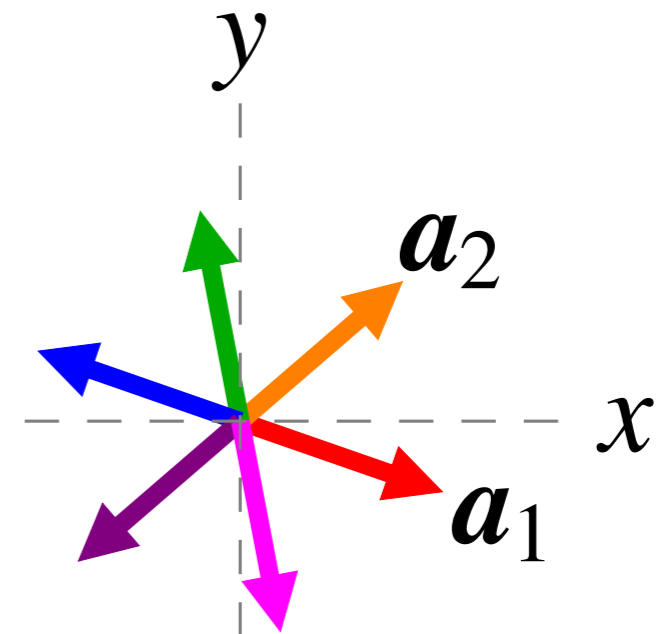
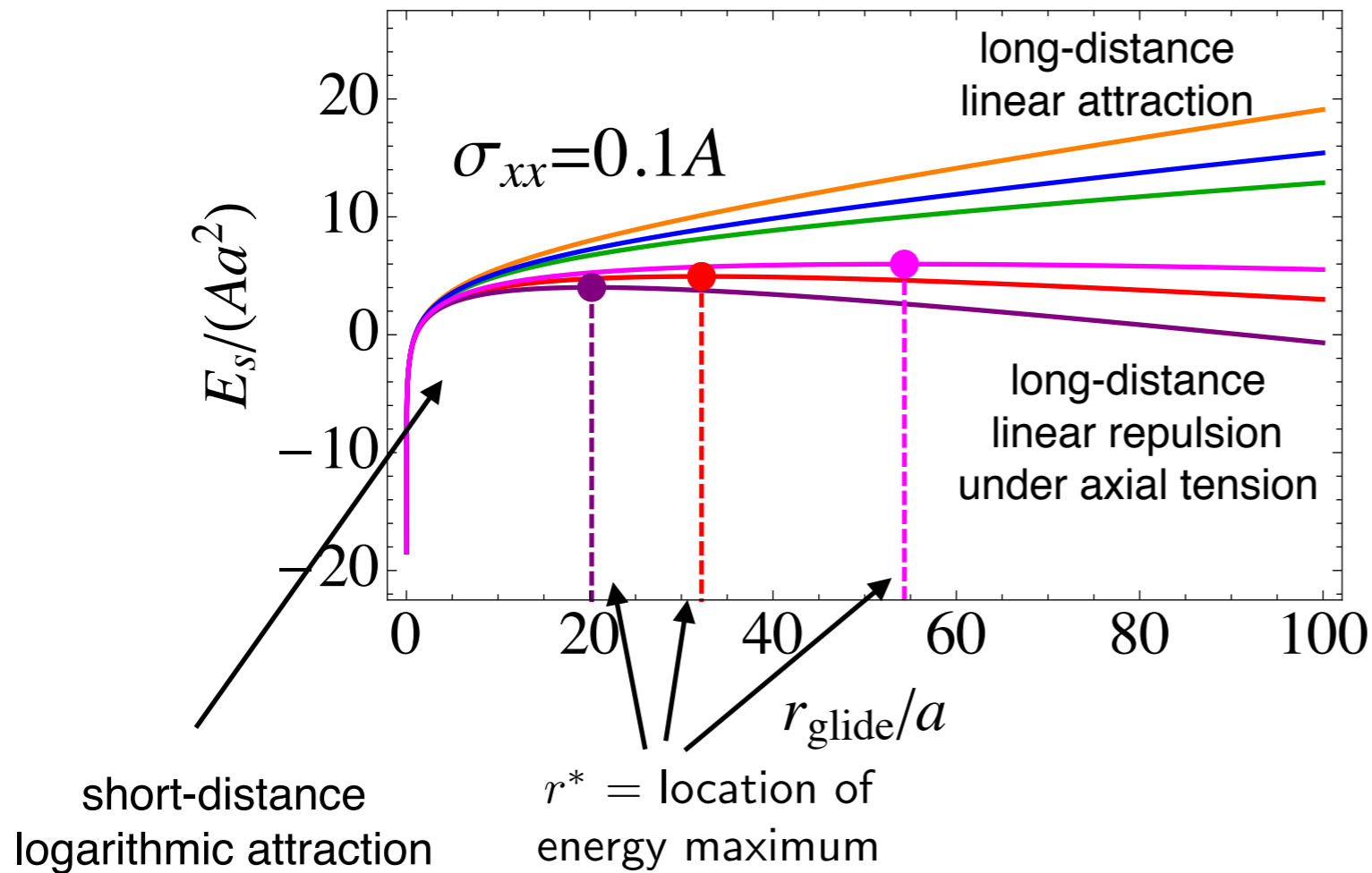
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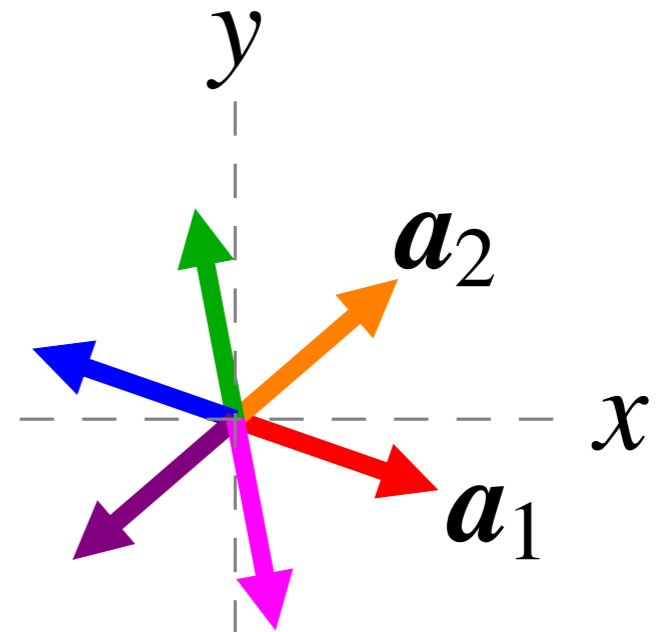
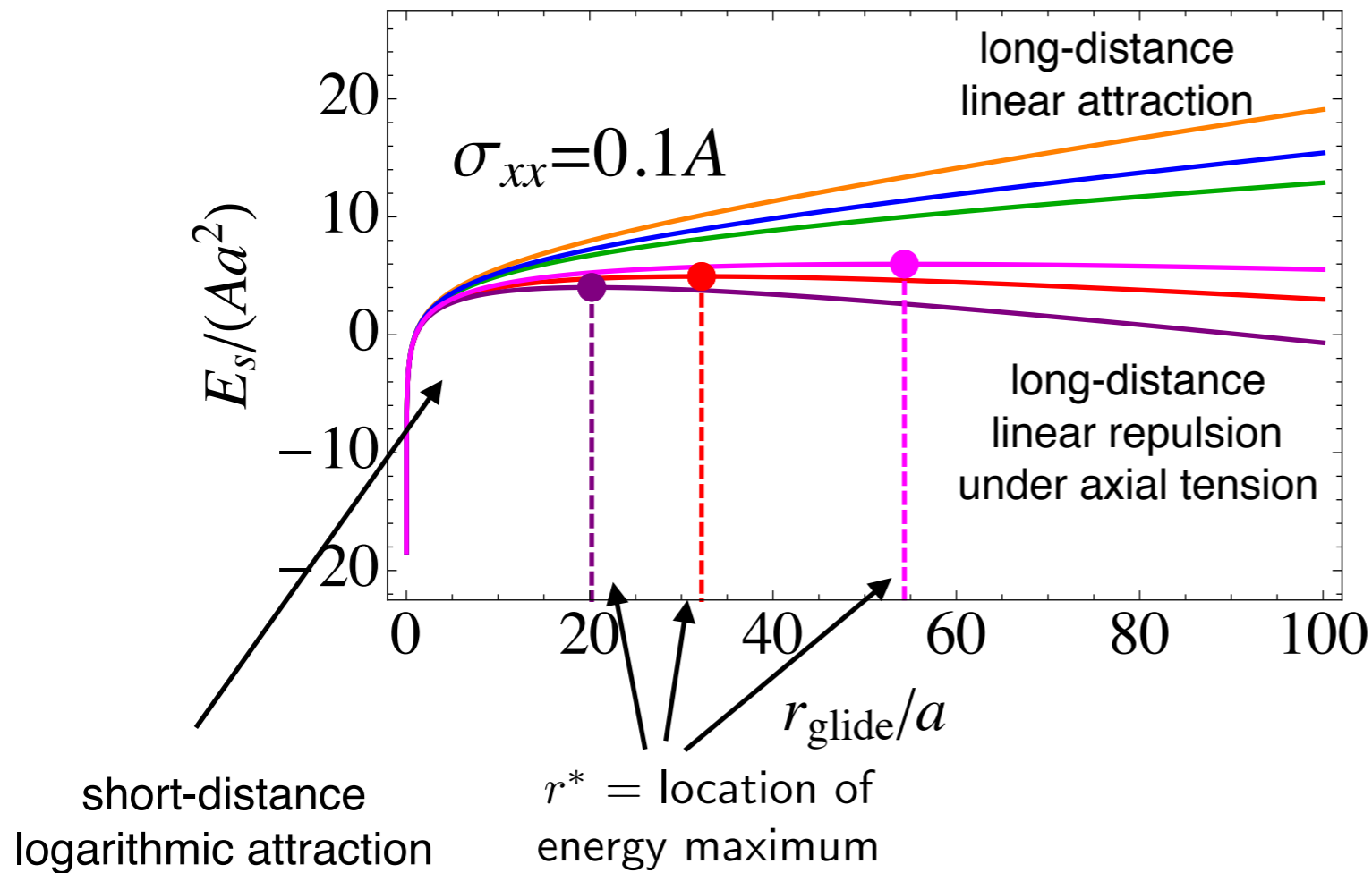
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Dislocation pair energy landscape

$$E_s(r) = Aa^2 \ln(r/a) + s \cdot a \cdot r \cdot \left[\frac{1}{2} \sin(2\theta) (\sigma_{xx}^{\text{ext}} - \sigma_{yy}^{\text{ext}}) - \cos(2\theta) \sigma_{xy}^{\text{ext}} \right] + \text{const.}$$

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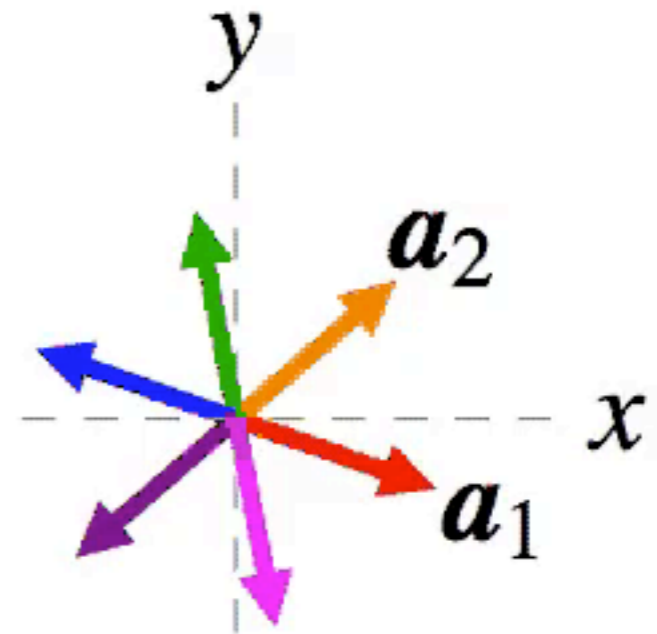
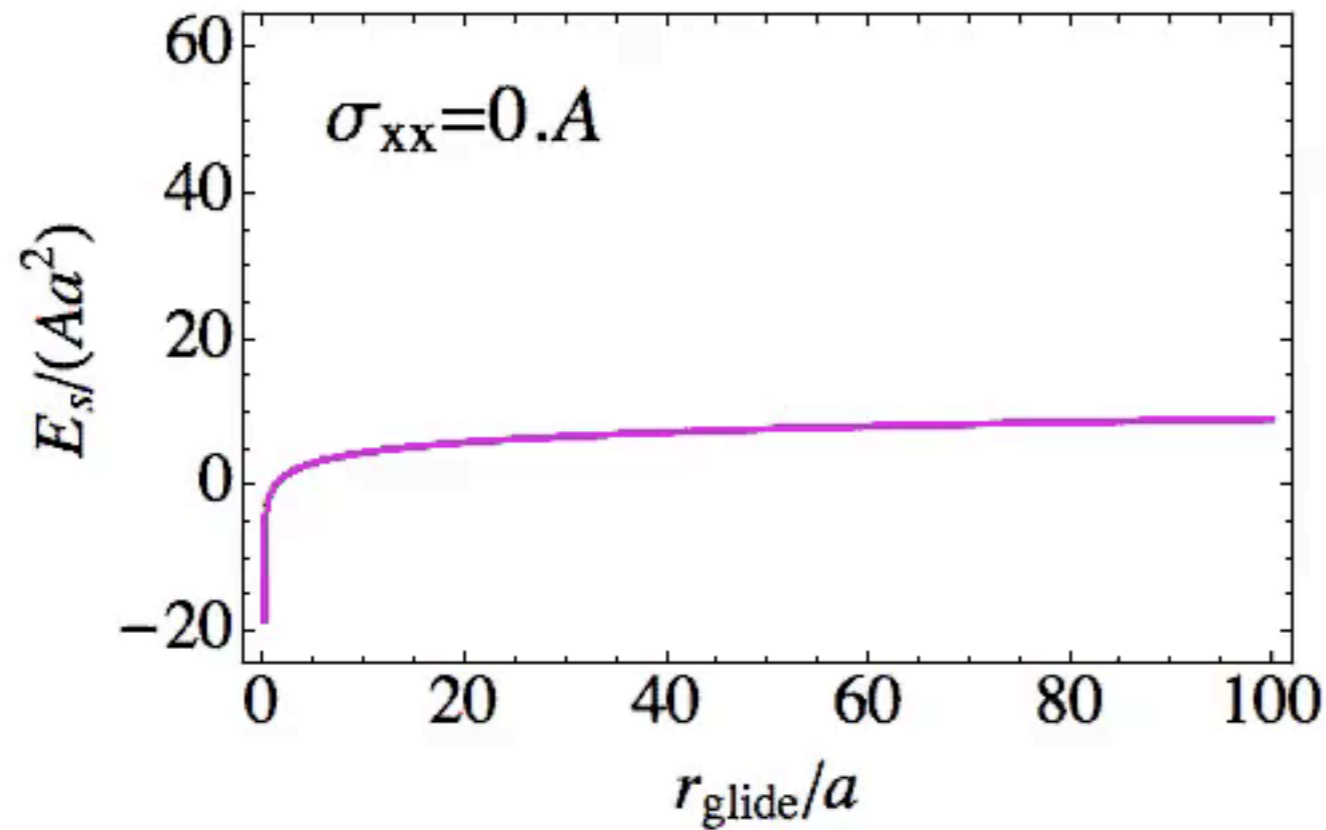
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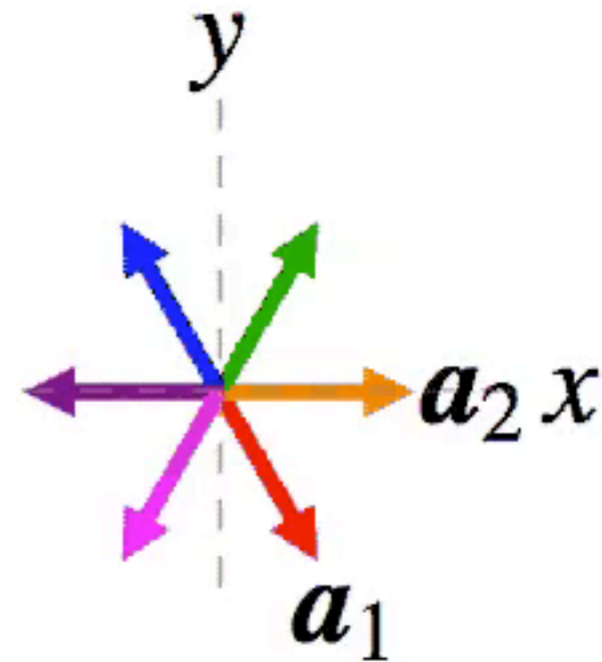
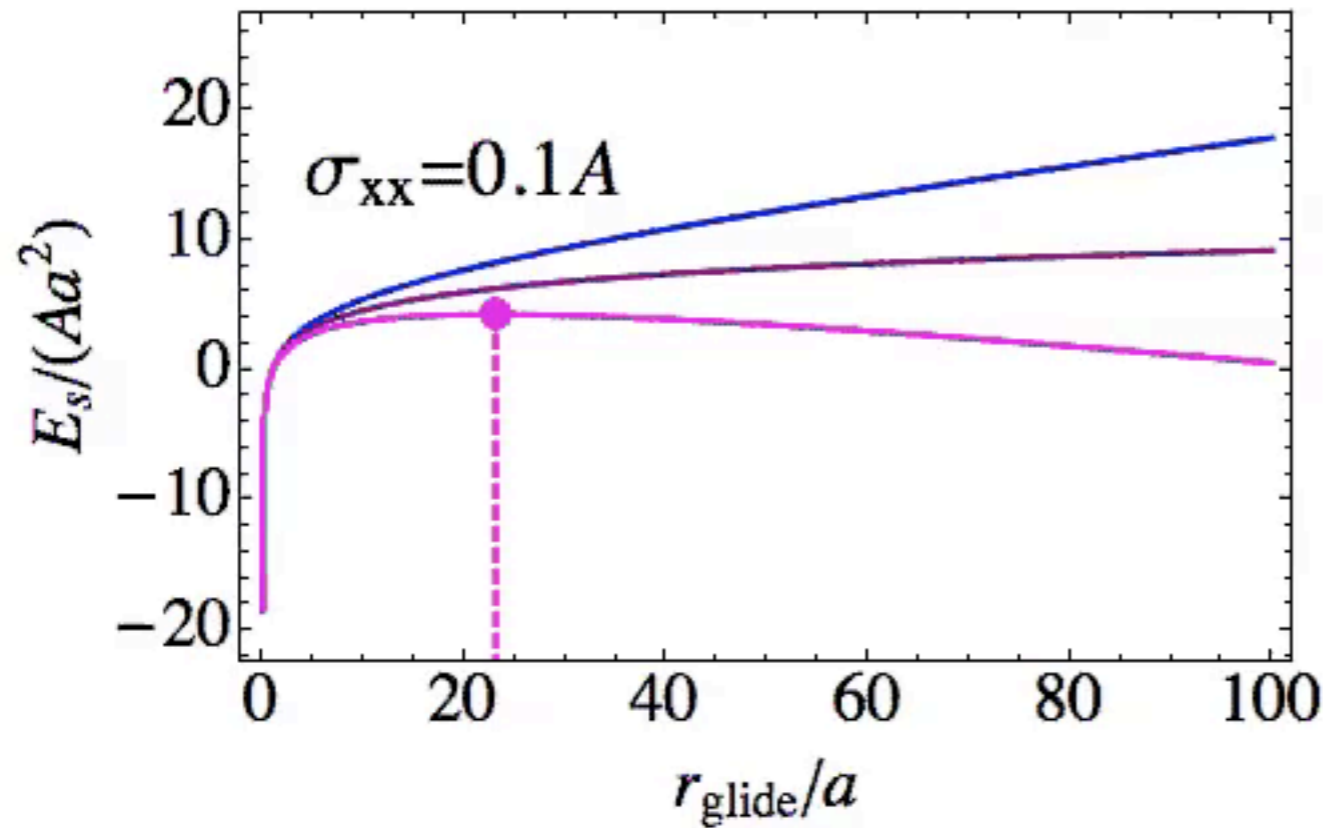
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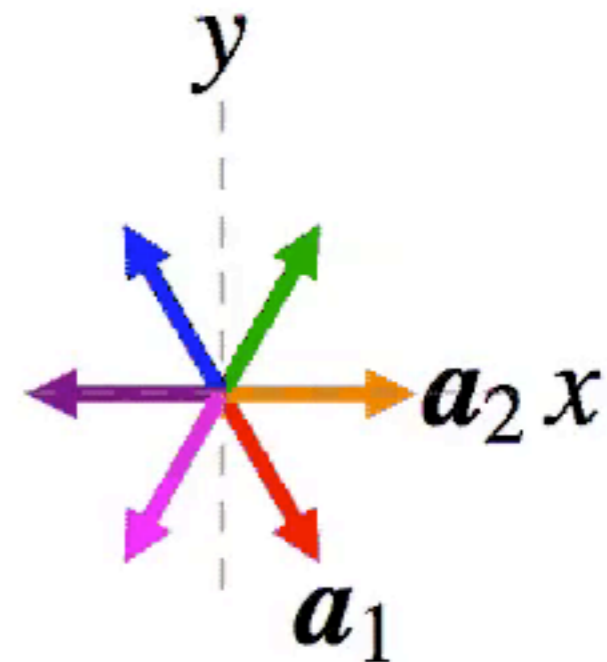
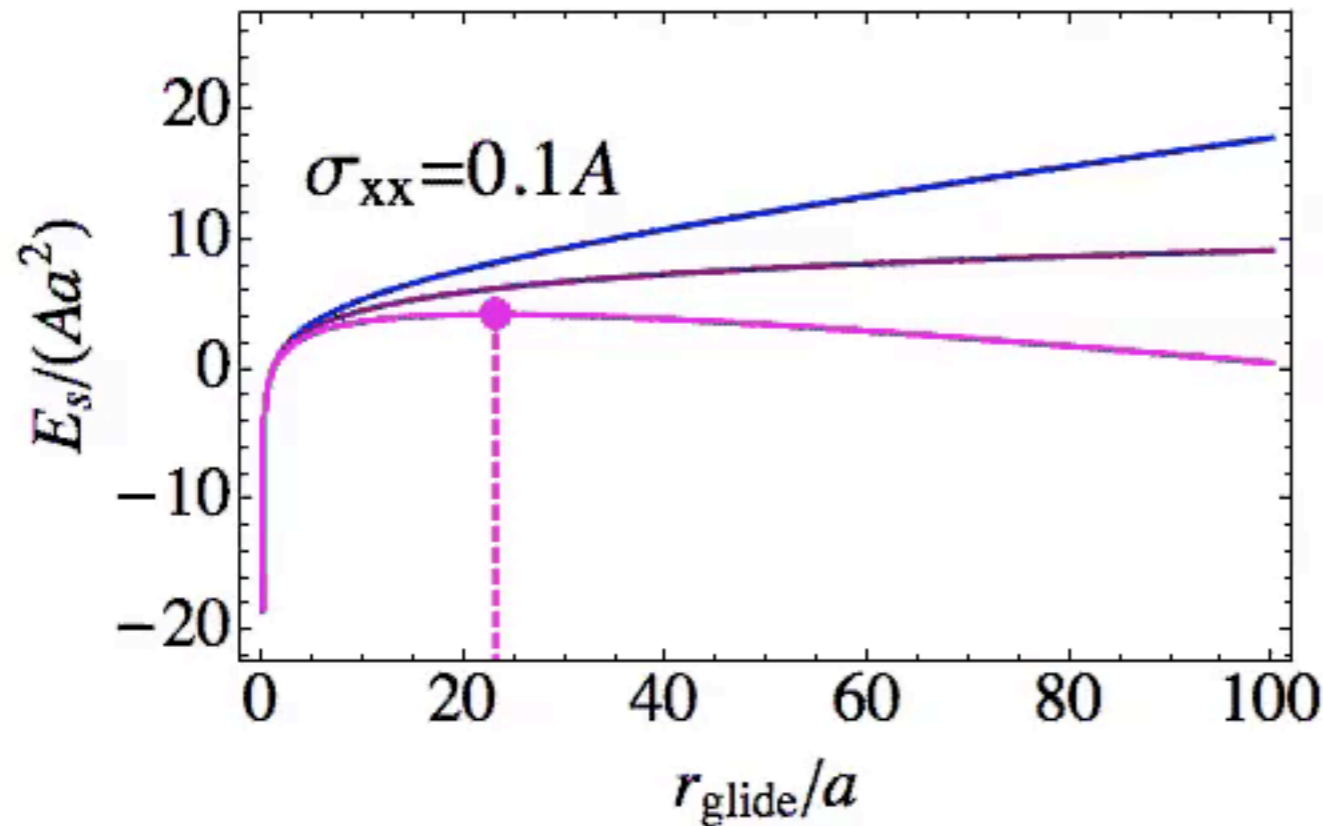


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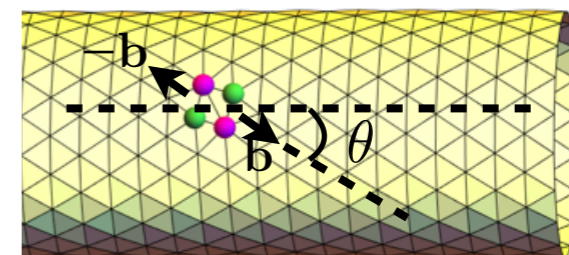
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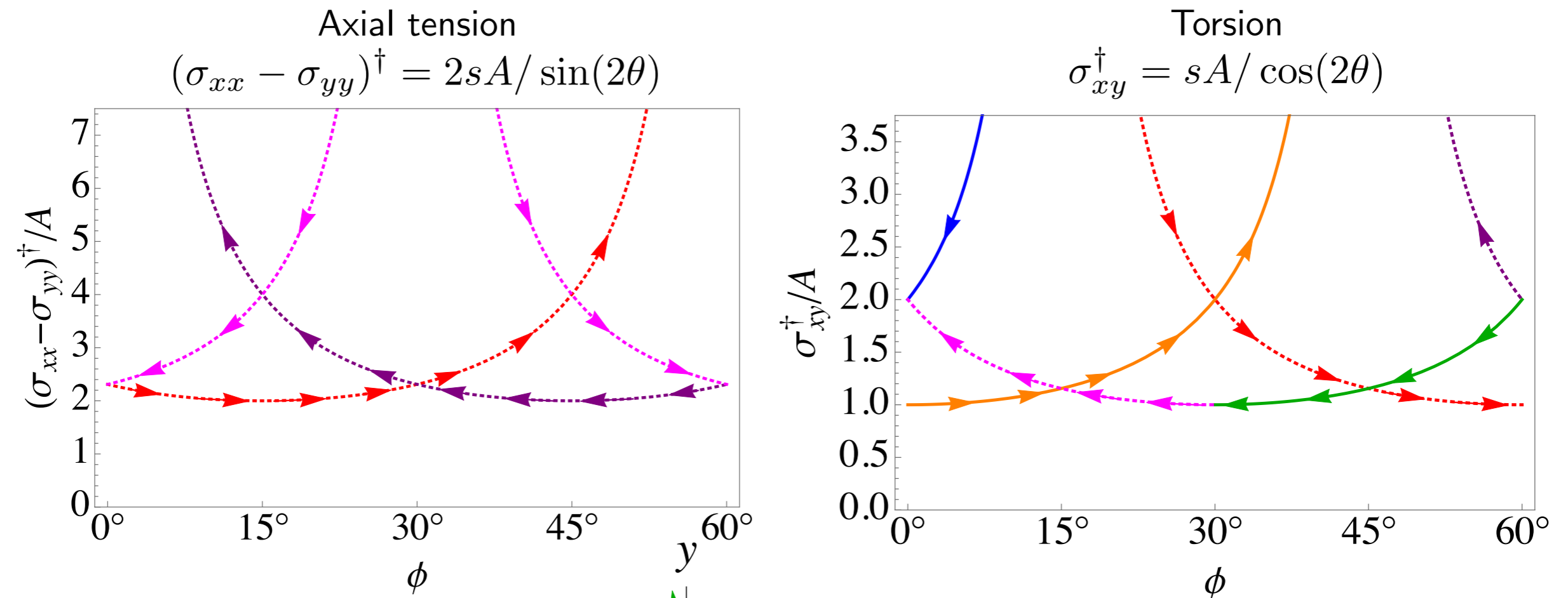
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Critical stress for plastic deformation of pristine lattice:
How strong must σ^{ext} be to make $r^* = a$?



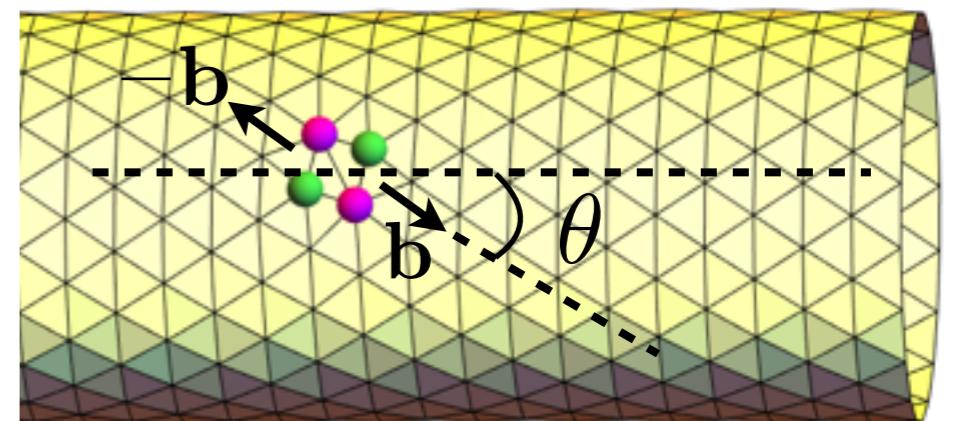
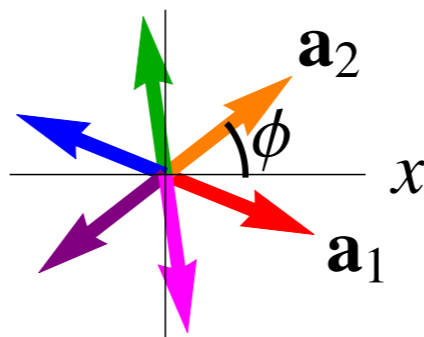
Critical stress required for instability to dislocation pair unbinding

Critical stress σ^\dagger to unbind an *elementary* dislocation pair ($|\mathbf{b}| = r = a$) and plastically deform the tube by dislocation glide:



Key:

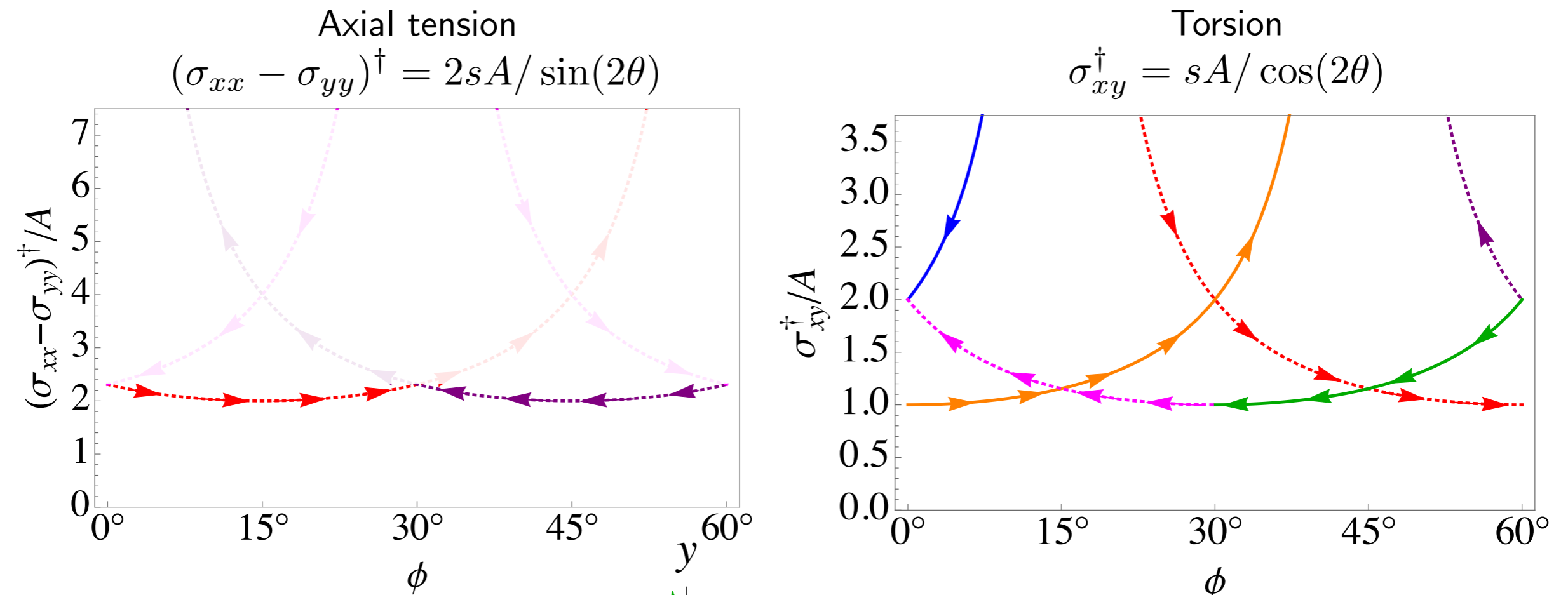
- increases R
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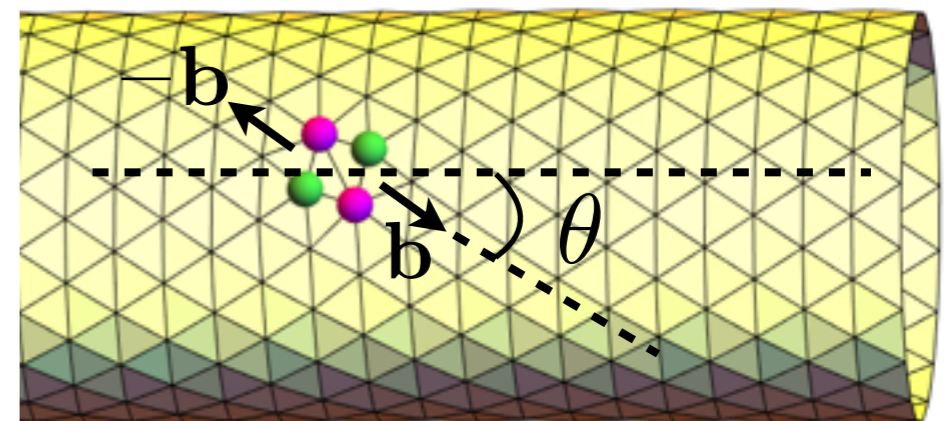
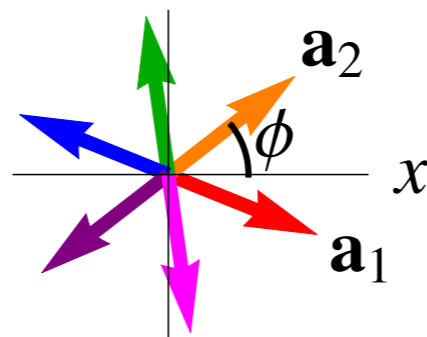
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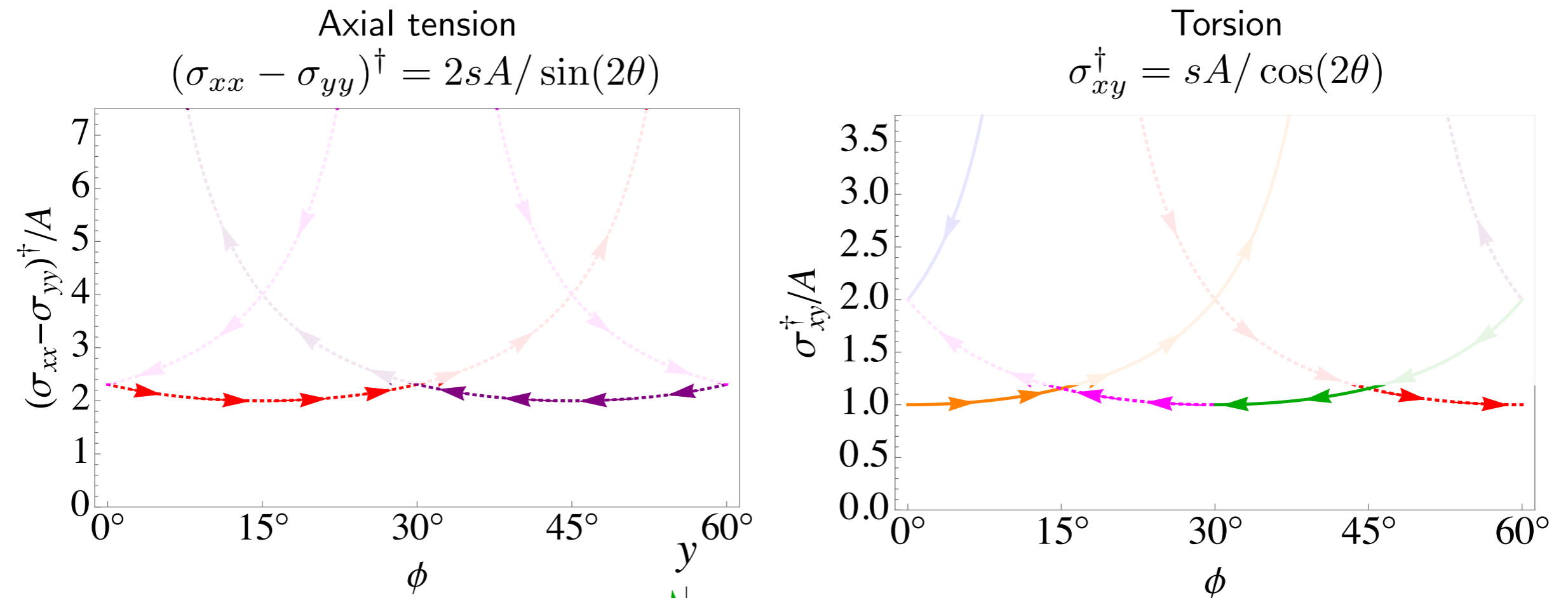
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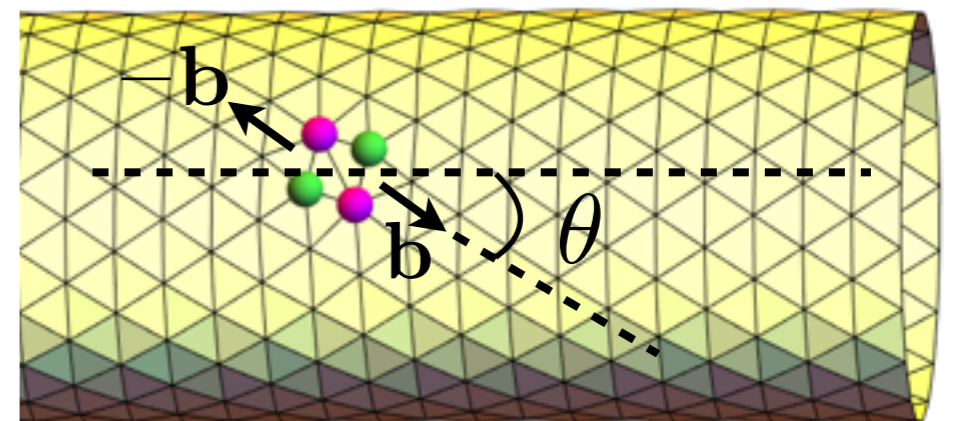
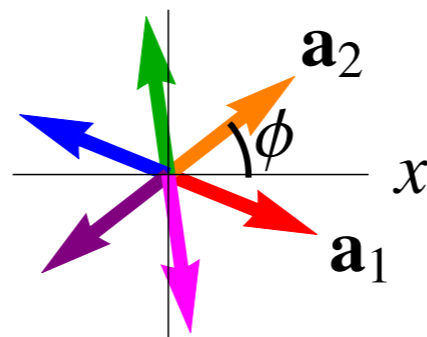
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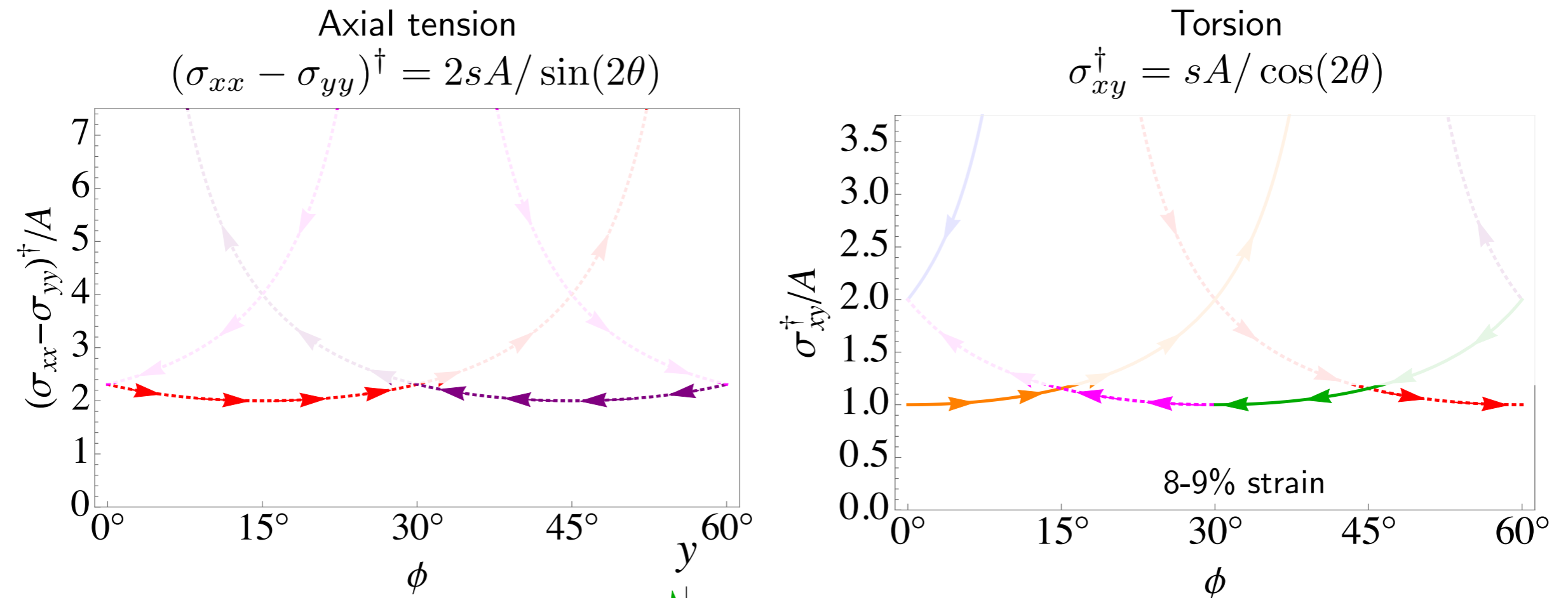
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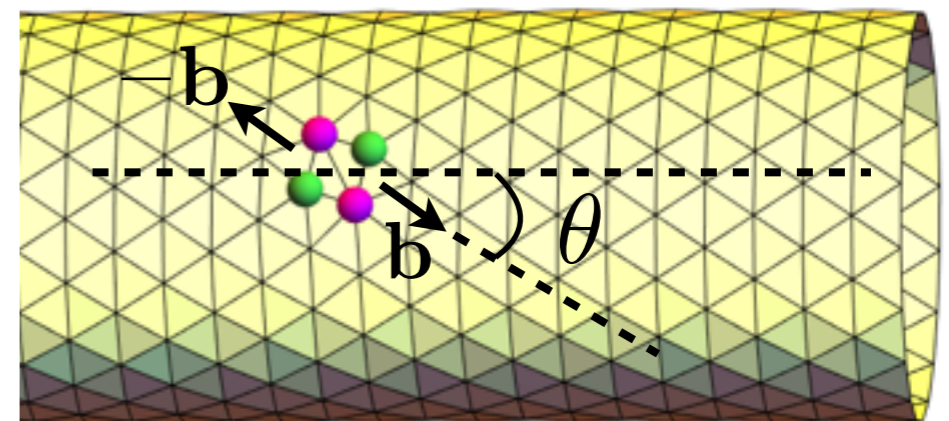
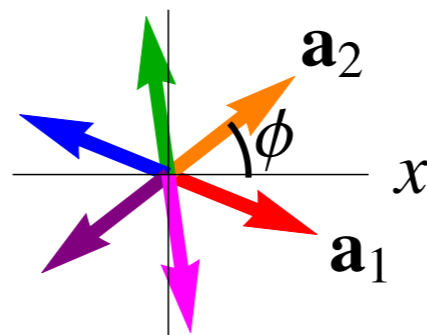
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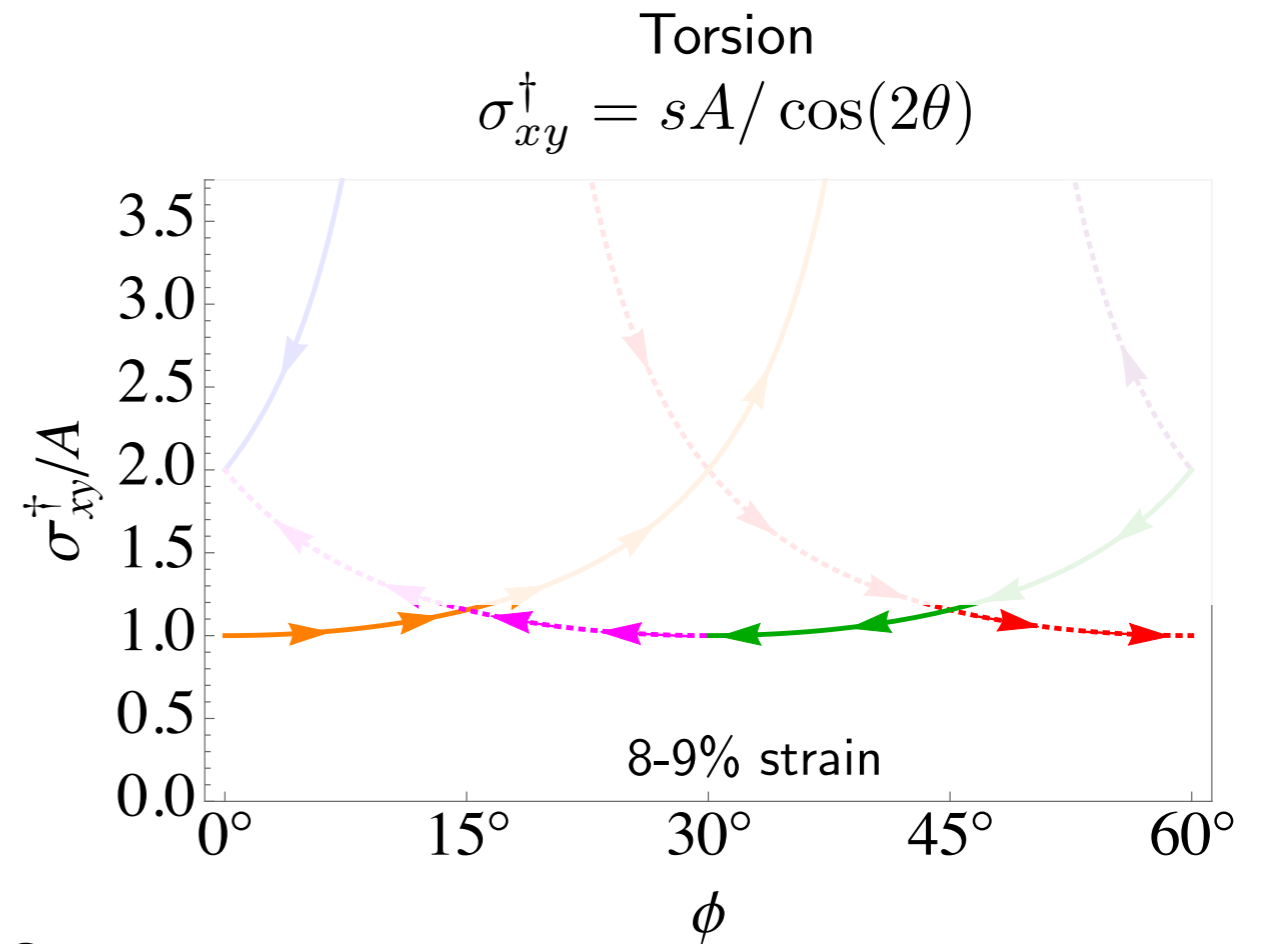
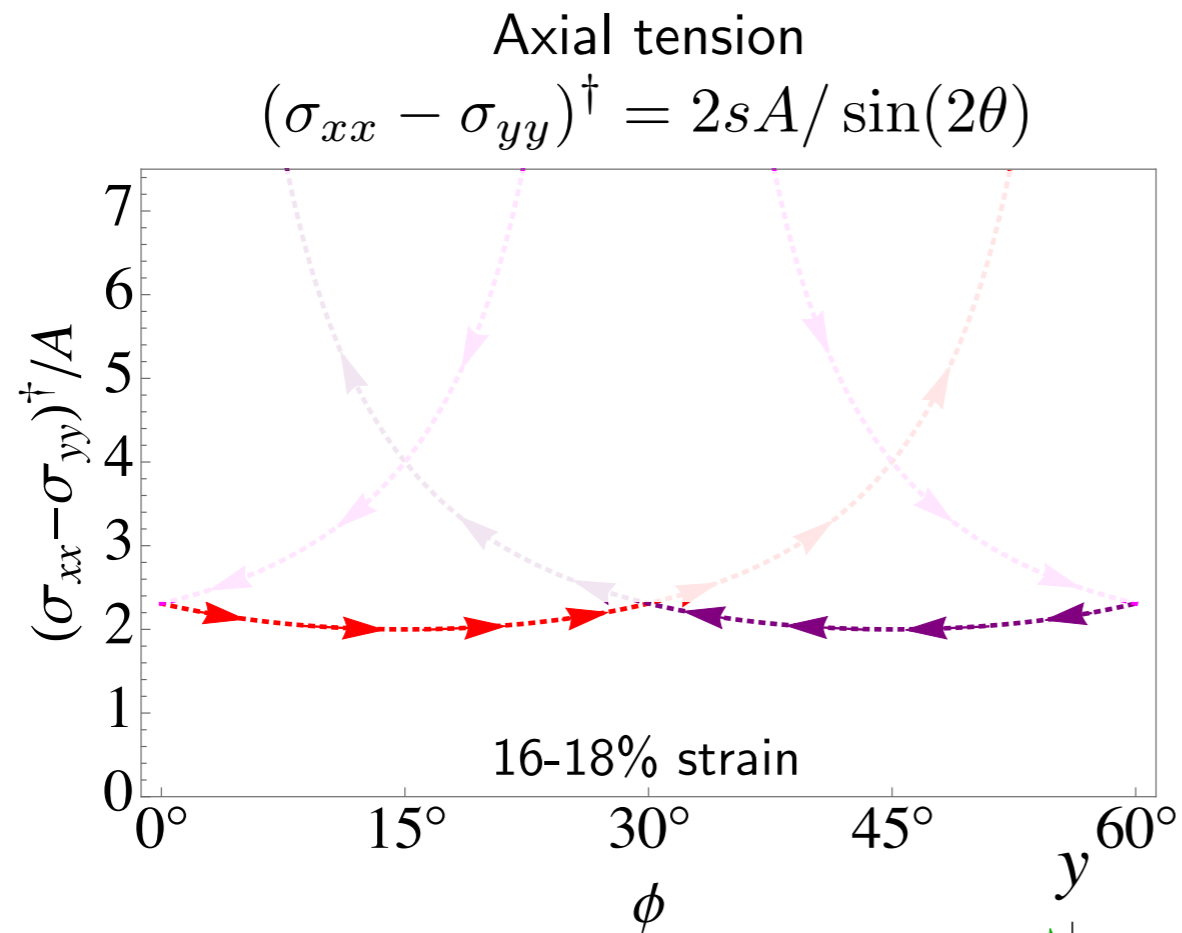
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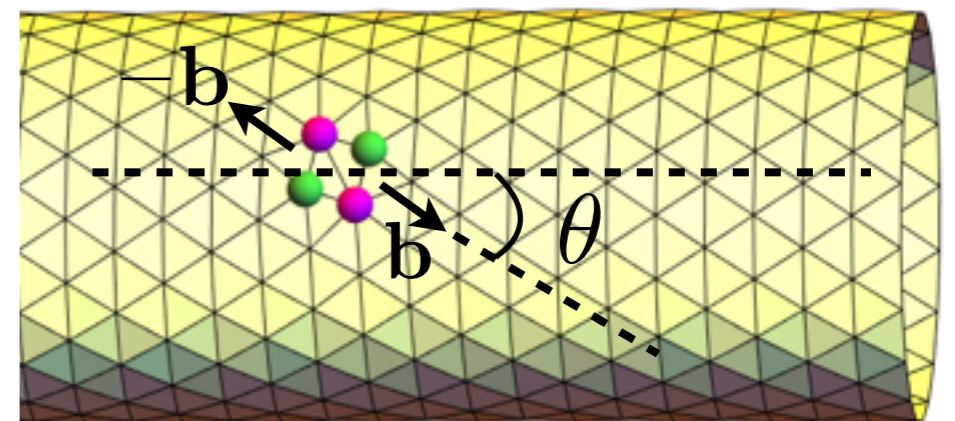
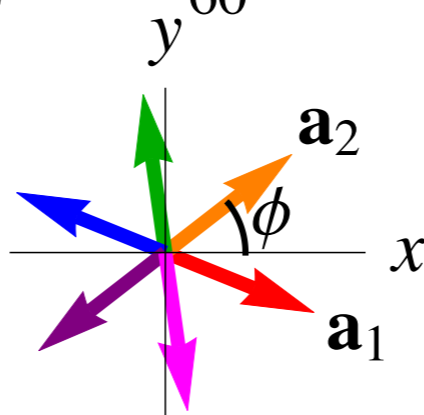
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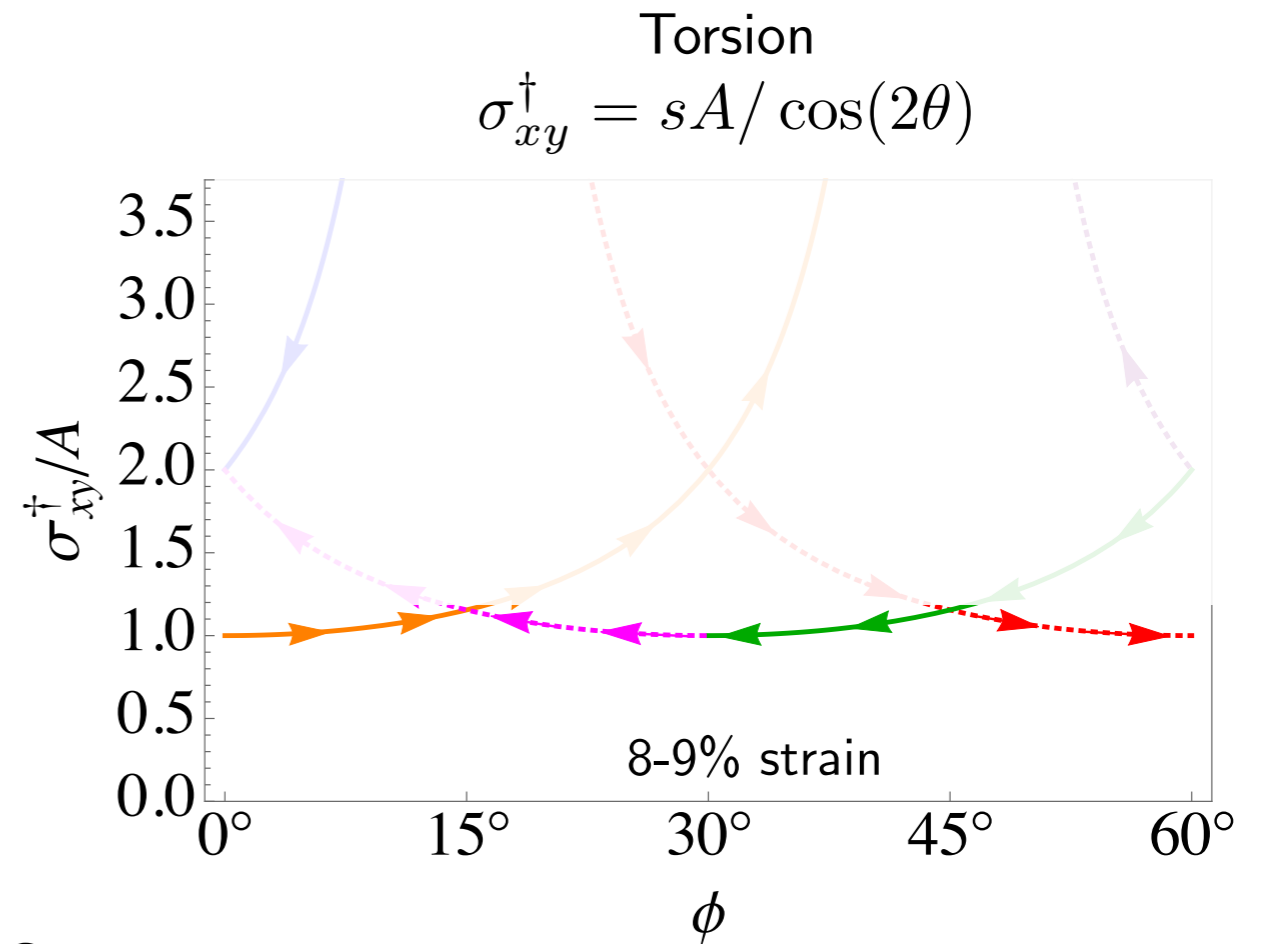
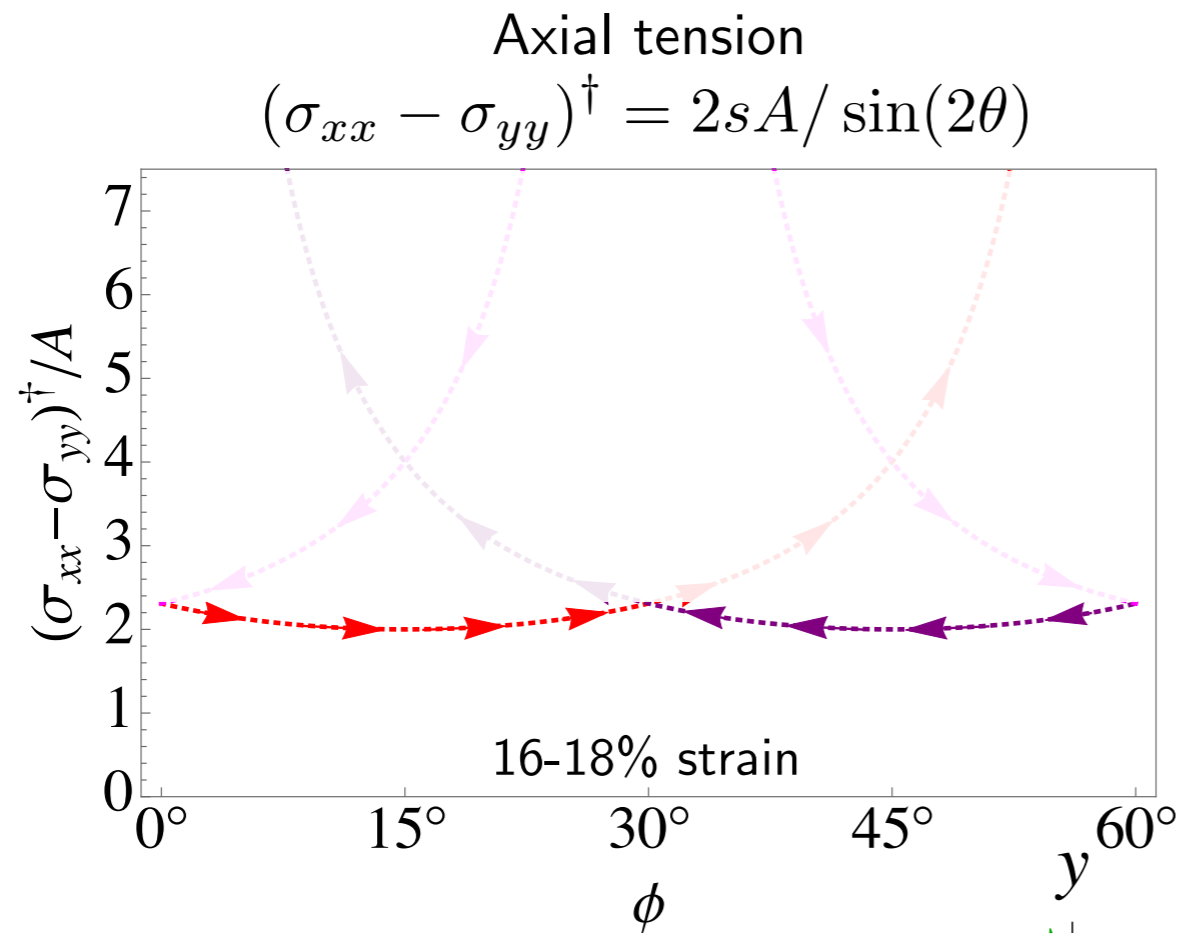
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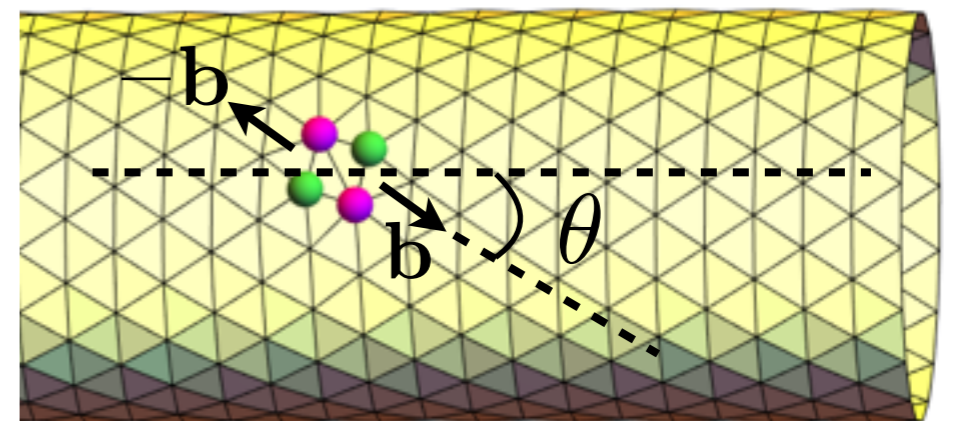
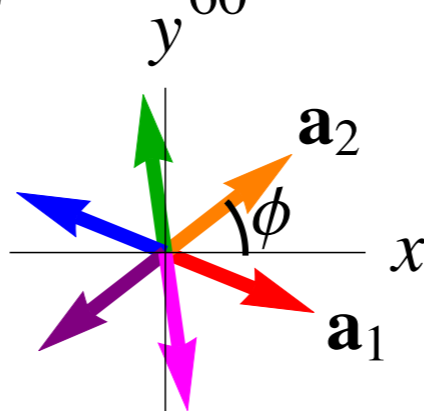
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So far we have only been considering planar dislocation interactions. How does being on a cylinder change defect interactions?

The bending energy

- Helfrich free energy for a bent membrane

$$E_b = \int d\mathbf{x} \left[\frac{1}{2} \kappa (H(\mathbf{x}))^2 + \bar{\kappa} K(\mathbf{x}) \right]$$

- Infinite cylinders/periodic B.C.'s $\Rightarrow \int d\mathbf{x} K(\mathbf{x}) = 0$.
- For a perfect cylinder, $H = 1/R$ so bending energy per unit length is $E_b/L = \pi \kappa / R$.

$$\begin{aligned} \text{Mean curvature } H &= \frac{1}{R_1} + \frac{1}{R_2} \\ \text{Gaussian curvature } K &= \frac{1}{R_1 R_2} \end{aligned}$$

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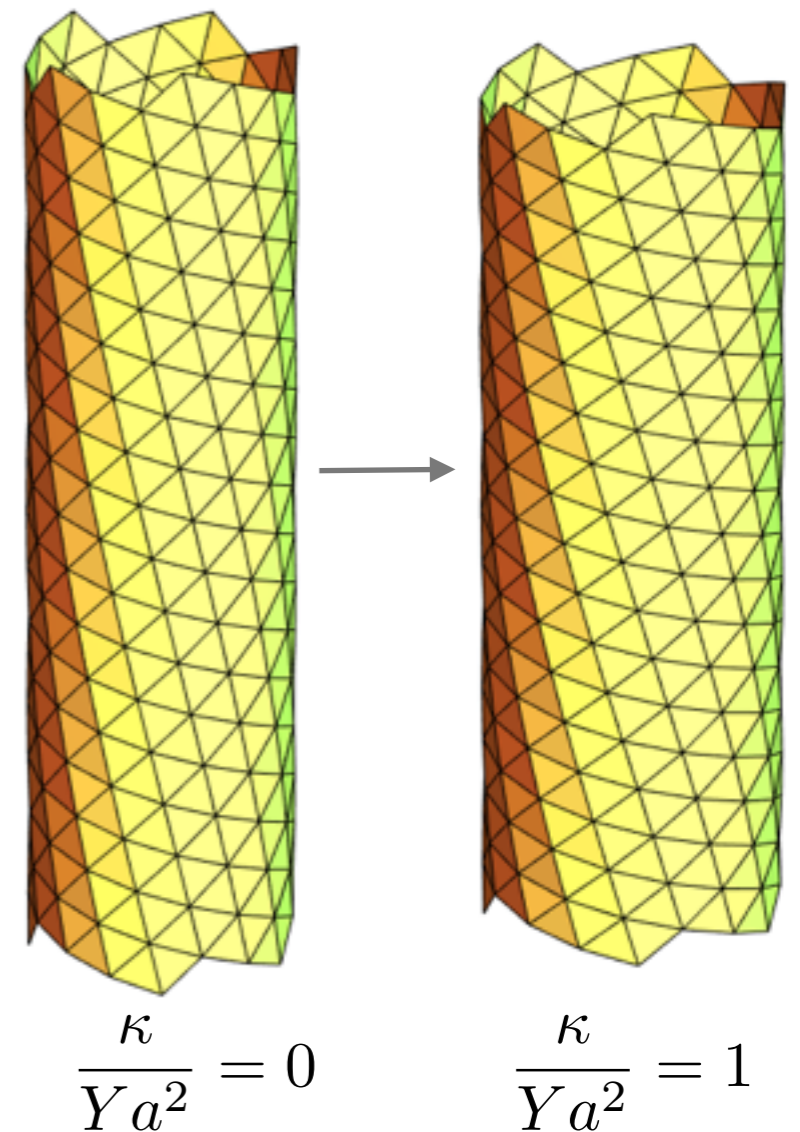
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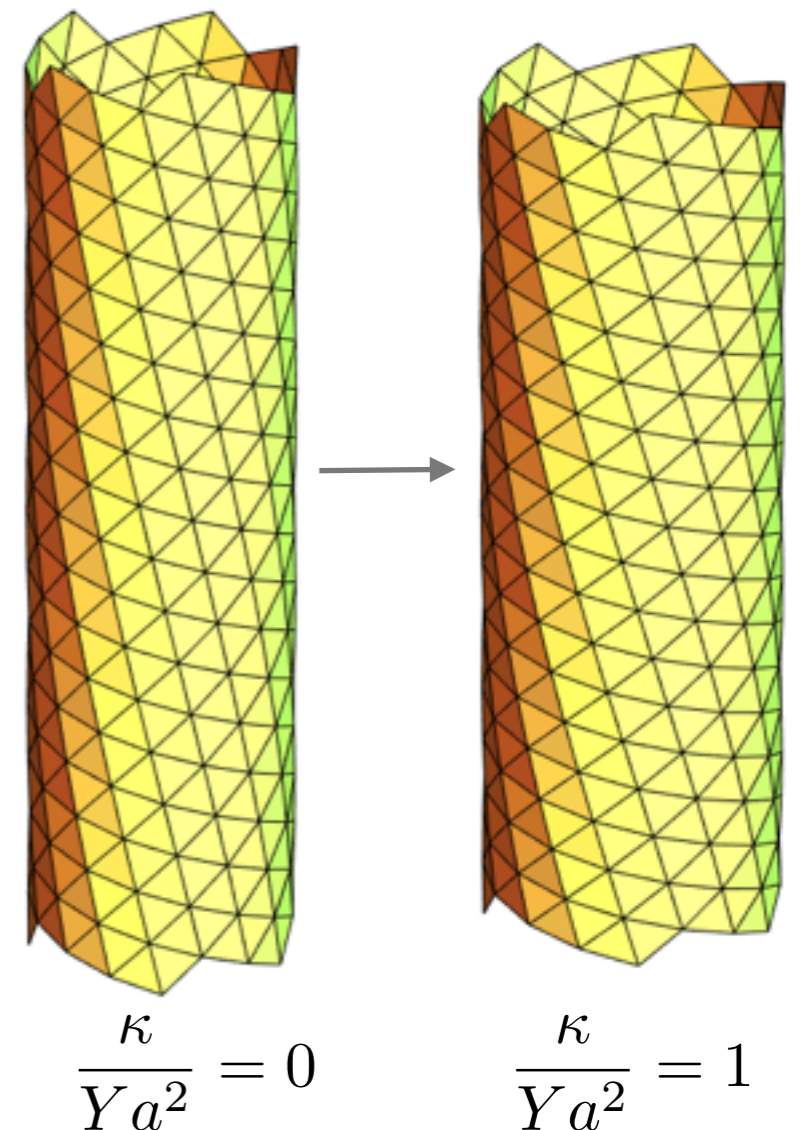
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- How important is bending energy E_b compared to stretching energy E_s ?
- Dimensionless ratio: the **Föppl-van Kármán number**

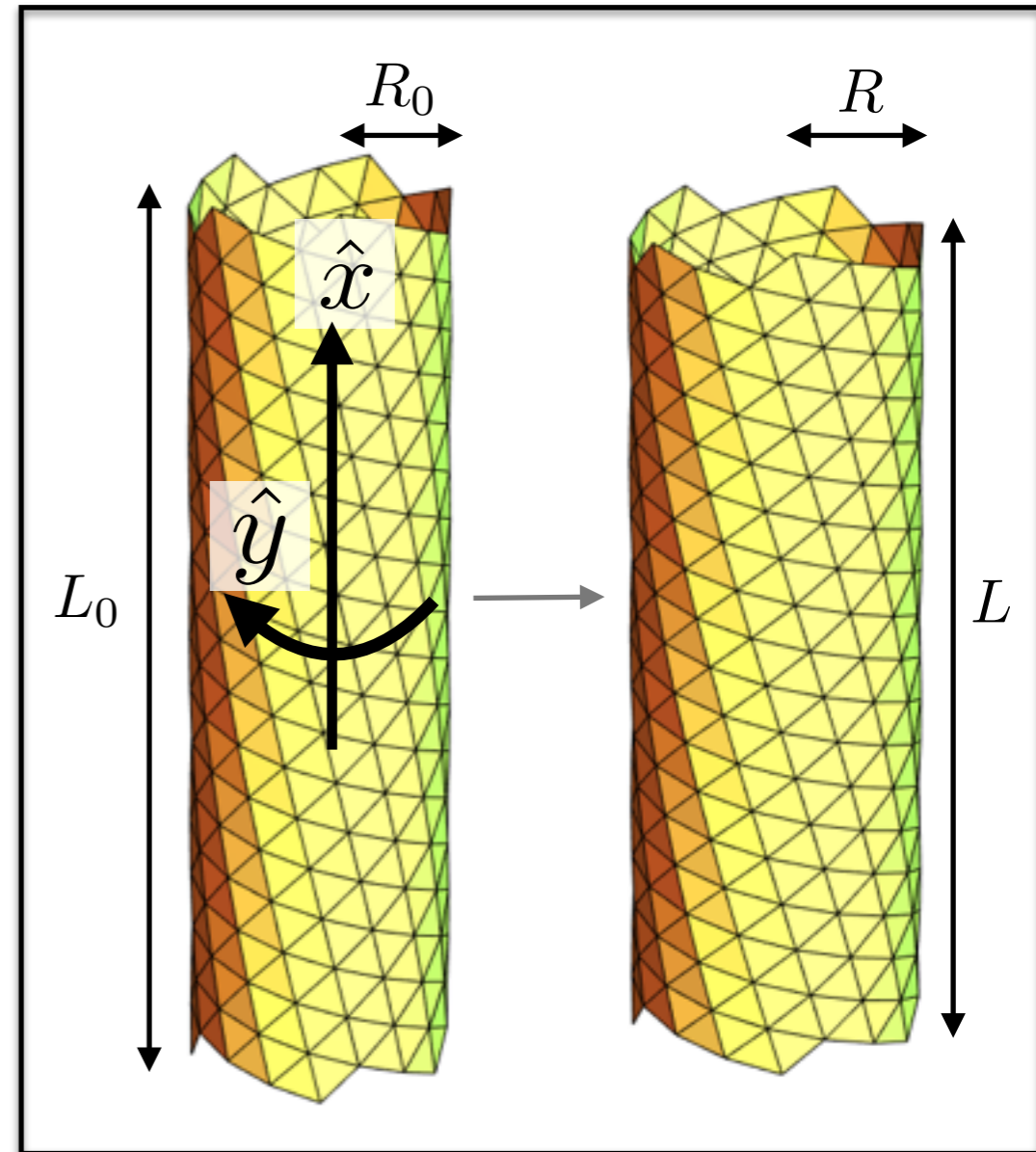
$$\gamma \equiv \frac{Y R^2}{\kappa}$$

- For large γ , bending is easier than stretching.
- *E.g.* For single-walled carbon nanotubes, $\gamma \sim 10^2 - 10^3$.



The bending energy as a perturbation

$$\text{Föppl-van Kármán number } \gamma \equiv \frac{Y R^2}{\kappa} \gg 1$$



The bending energy as a perturbation

- Radius preferred by stretching energy:

$$R_0 \approx \frac{a}{2\pi} \sqrt{m^2 + n^2 - mn}$$

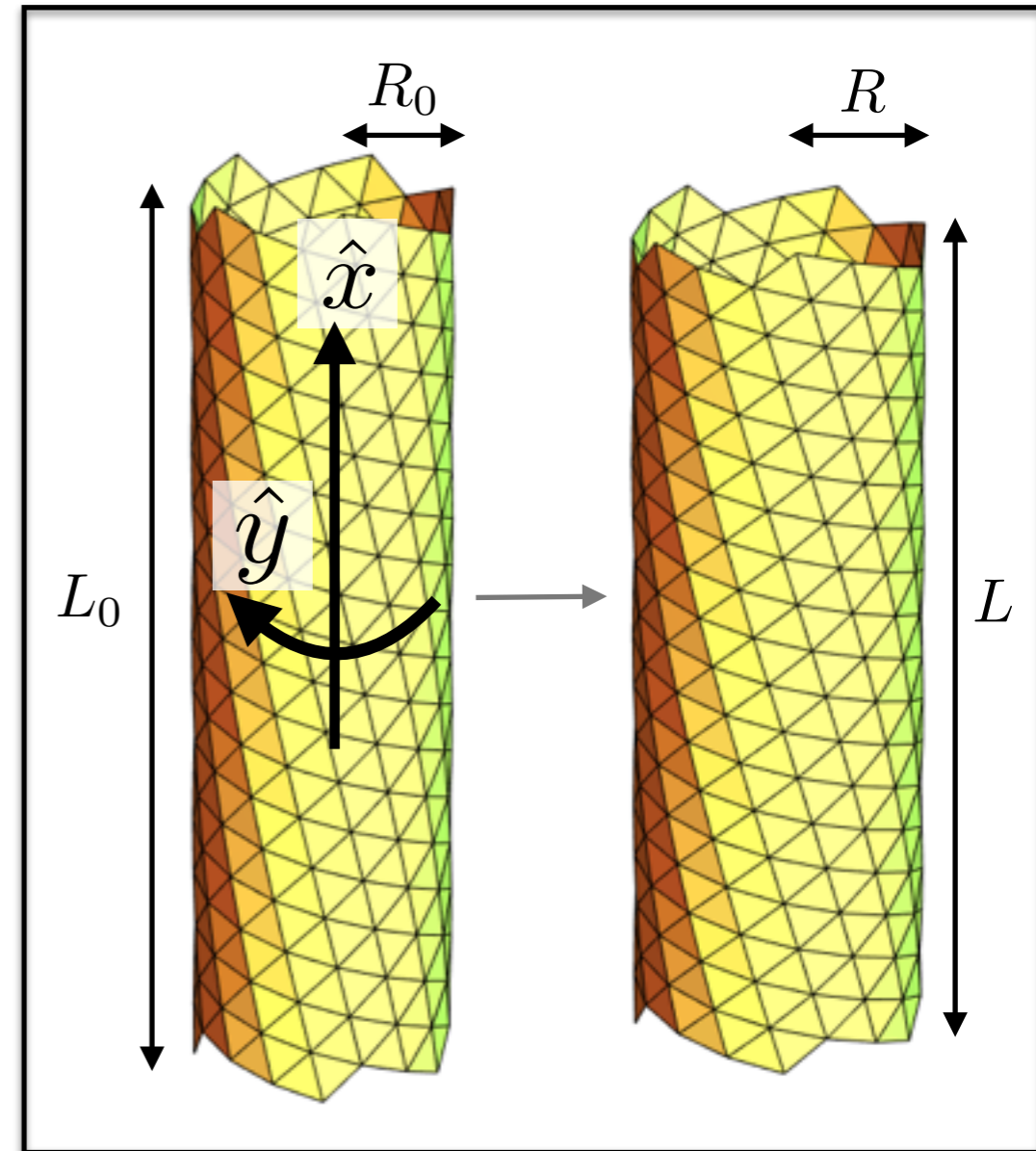
- With stretching *and* bending energies,

$$L_0 \rightarrow L = L_0(1 + u_{xx})$$

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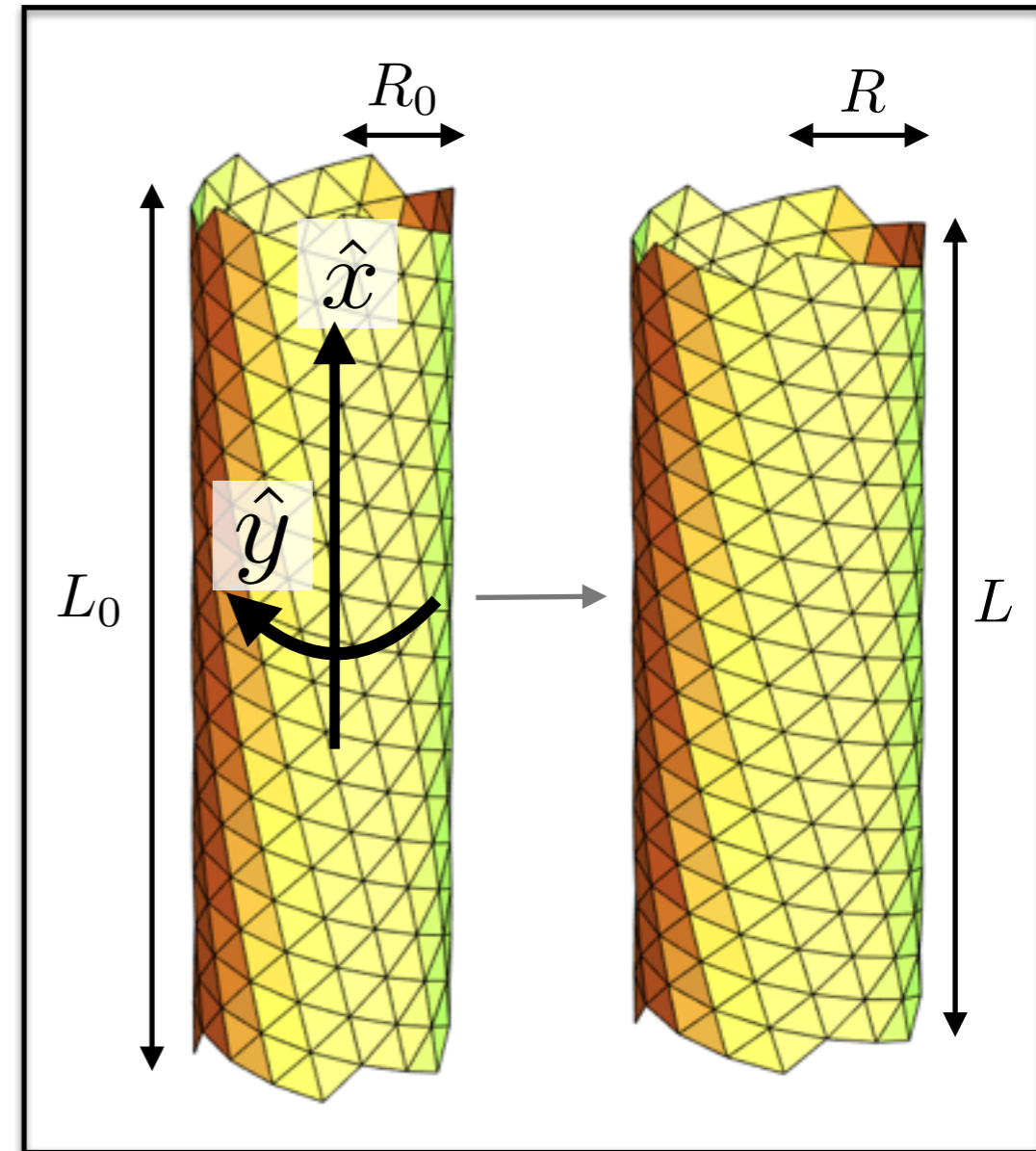
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$$= \frac{1}{2} \cdot \frac{3}{8} Y \int d\mathbf{x} (2u_{ij}u_{ij} + u_{kk}^2) + \frac{1}{2} \kappa \int d\mathbf{x} R^{-2}$$

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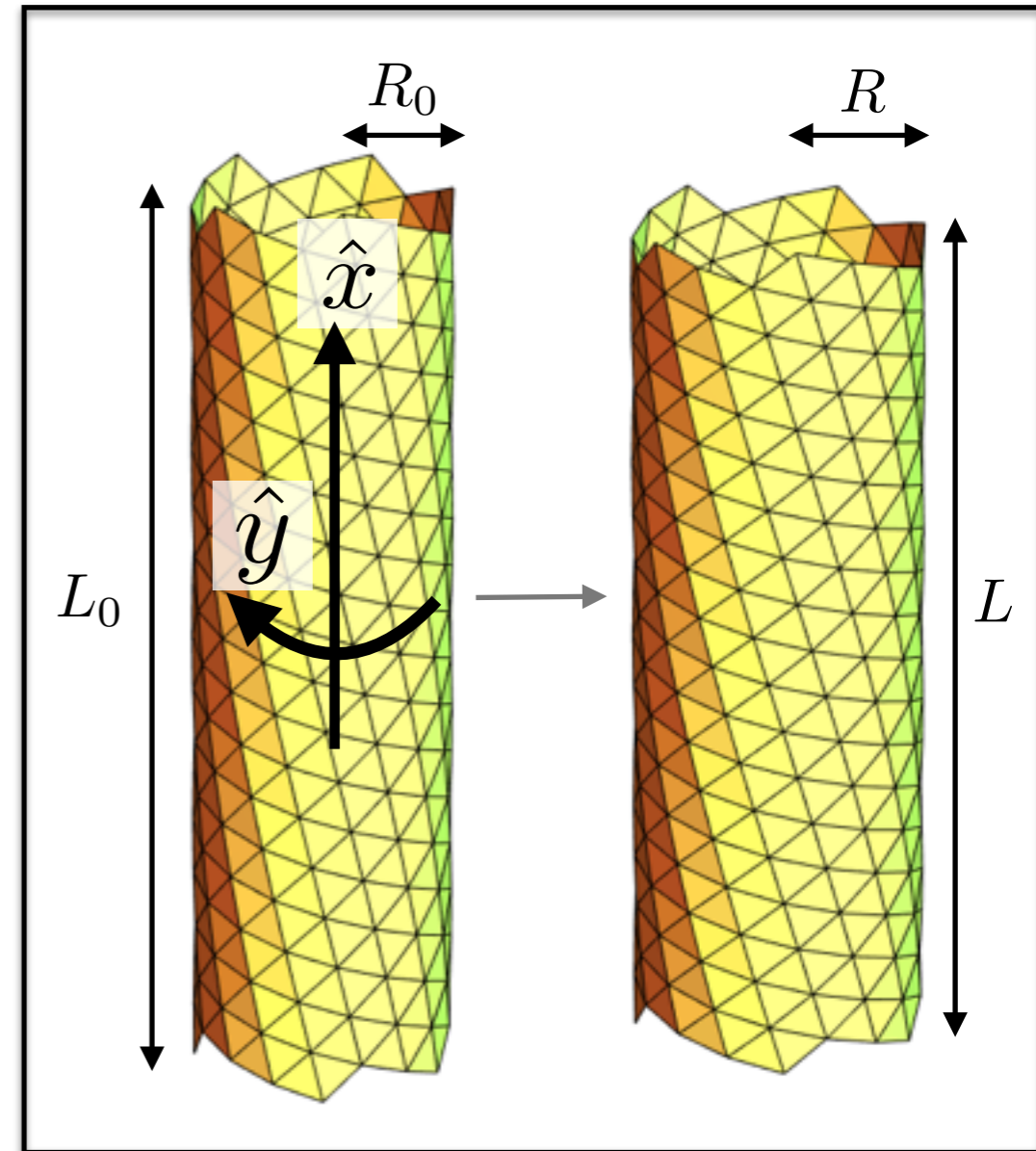
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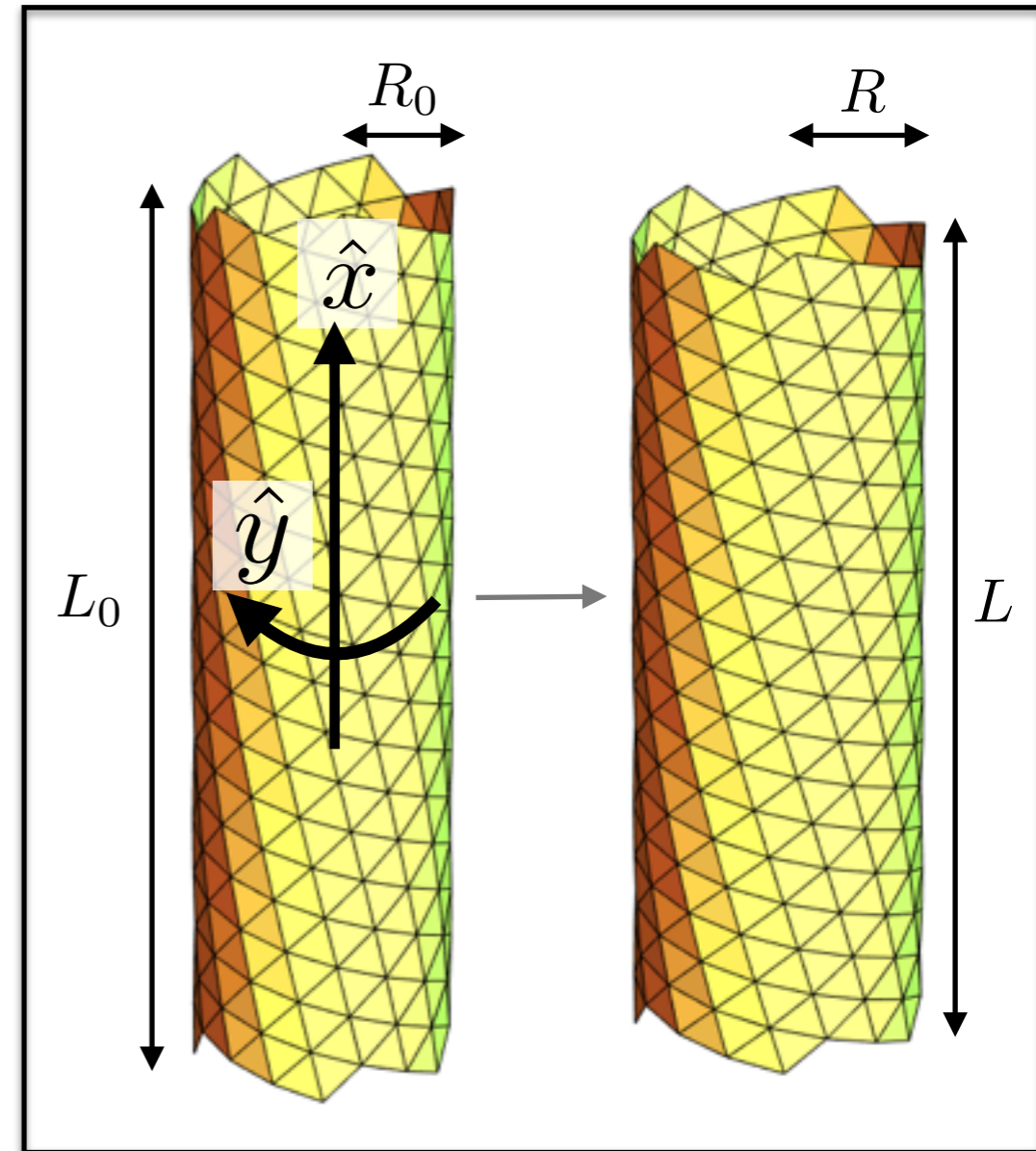
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γ^{-1}



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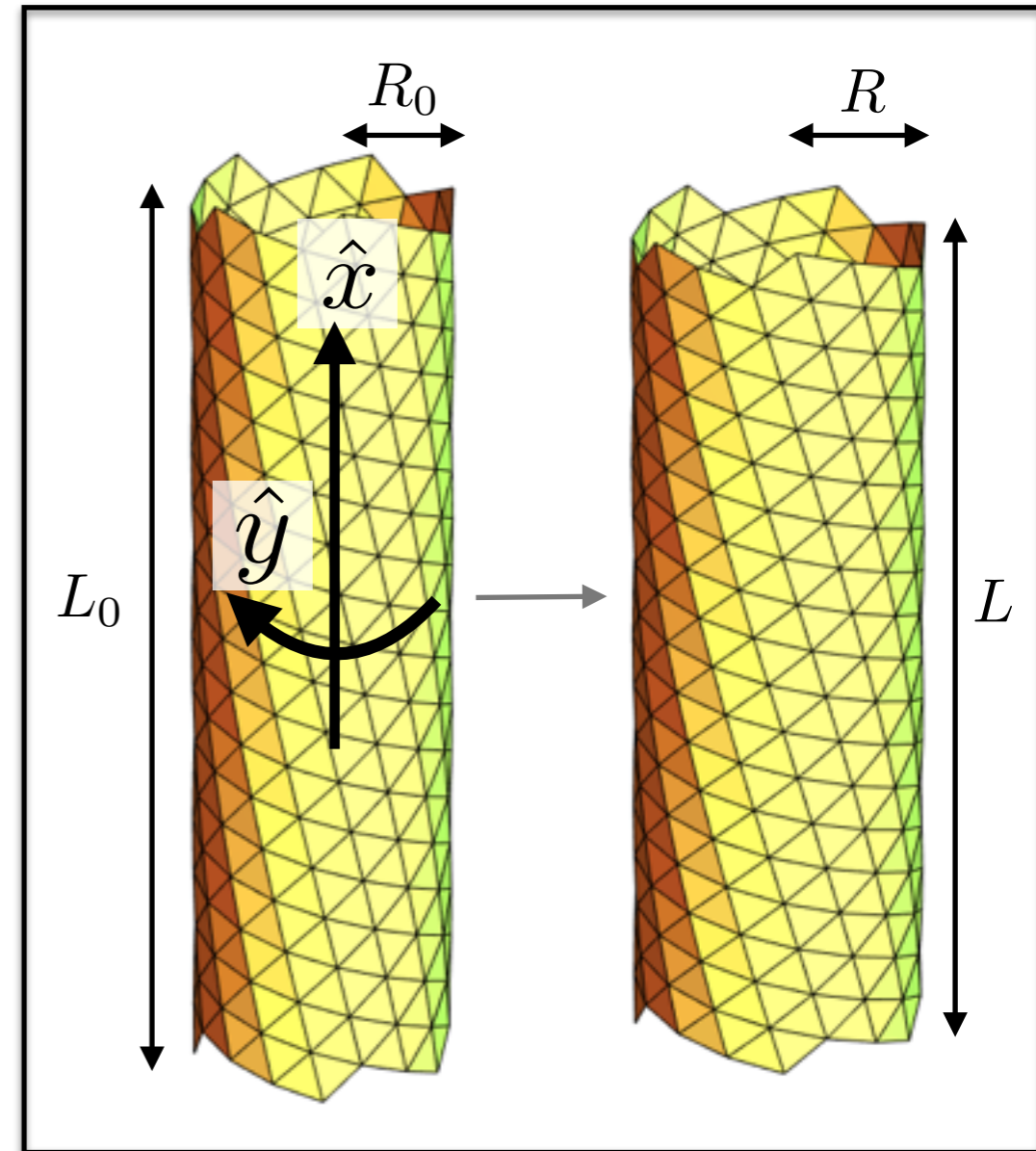
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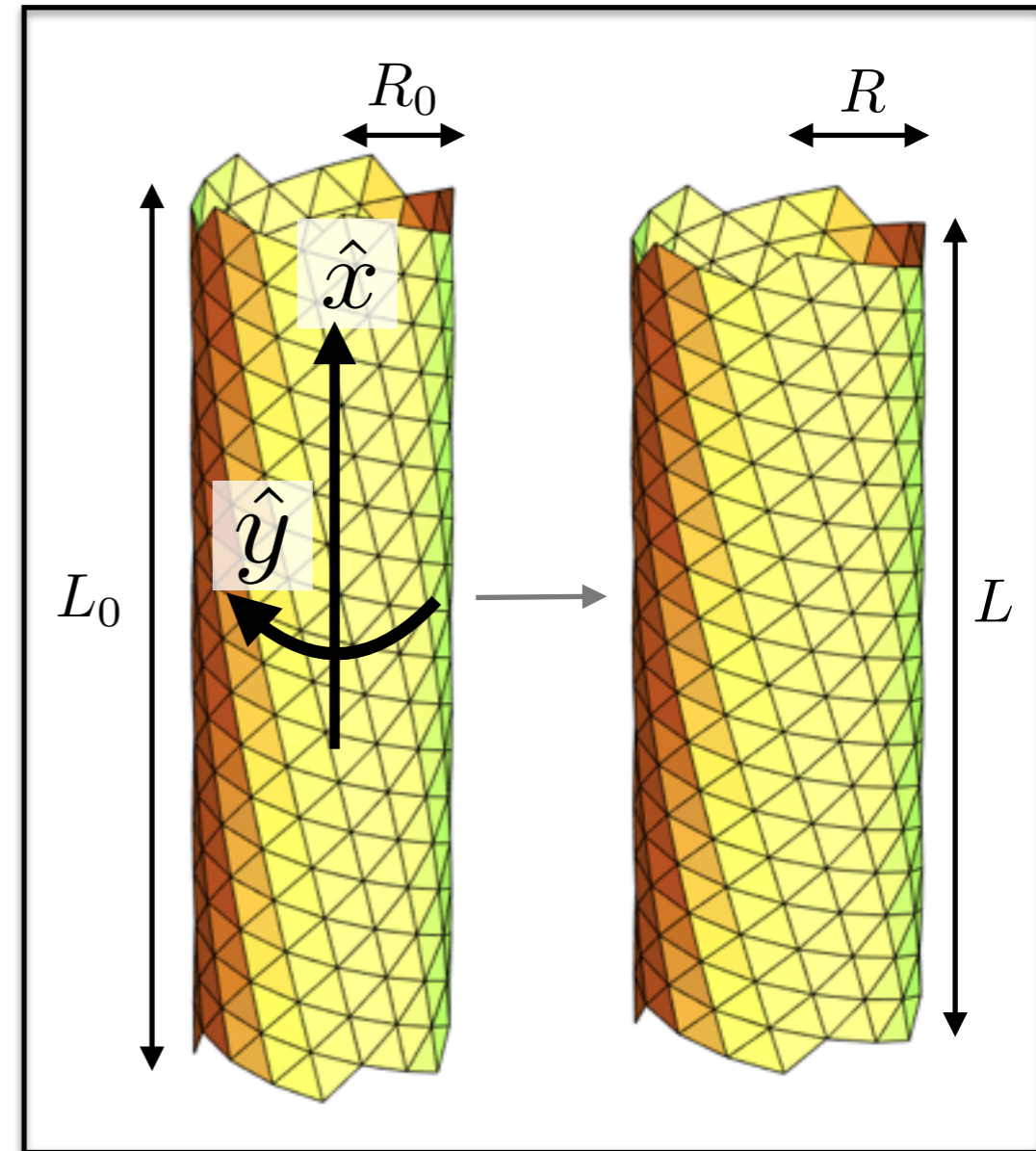
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E_b preserves area:
 $L \times R = L_0 \times R_0$

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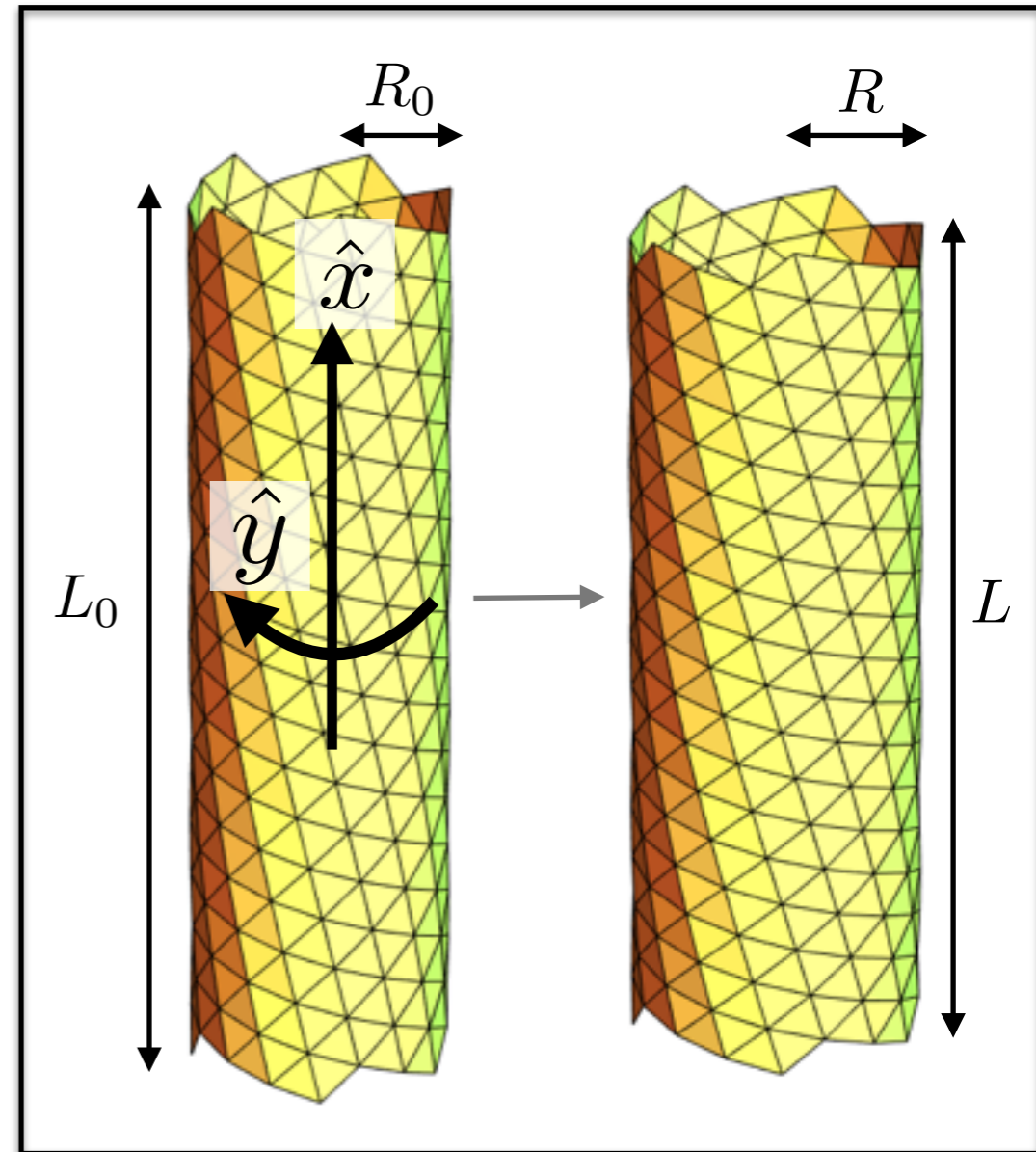
$$R_0 \rightarrow R = R_0(1 + u_{yy})$$

- Expand $E_{\text{tot}} = E_s + E_b$ in small γ^{-1} , u_{xx} , and u_{yy} .

$$\begin{aligned} E_{\text{tot}} &= E_s + E_b \\ &= \frac{1}{2} \cdot \frac{3}{8} Y \int d\mathbf{x} (2u_{ij}u_{ij} + u_{kk}^2) + \frac{1}{2} \kappa \int d\mathbf{x} R^{-2} \\ &= \frac{1}{2} \cdot \frac{3}{8} Y (2\pi R L) [2(u_{xx}^2 + u_{yy}^2) + (u_{xx} + u_{yy})^2] + \frac{\pi \kappa L}{R} \\ &\approx \pi Y R_0 L_0 \left[\frac{3}{8} (3u_{xx}^2 + 3u_{yy}^2 + 2u_{xx}u_{yy}) + \frac{\kappa}{Y R_0^2} (1 + u_{xx} - u_{yy}) \right] \end{aligned}$$

E_b preserves area:
 $L \times R = L_0 \times R_0$

$$\partial E_{\text{tot}} / \partial u_{xx} = \partial E_{\text{tot}} / \partial u_{yy} = 0 \Rightarrow u_{yy} = -u_{xx} \approx \frac{2}{3} \gamma^{-1} \Rightarrow R \approx R_0 \left(1 + \frac{2}{3} \gamma^{-1} \right)$$



The bending energy as an effective stress

- $u_{yy} = -u_{xx} \approx \frac{2}{3}\gamma^{-1}$
- Bending energy has same effect as an external stress tensor

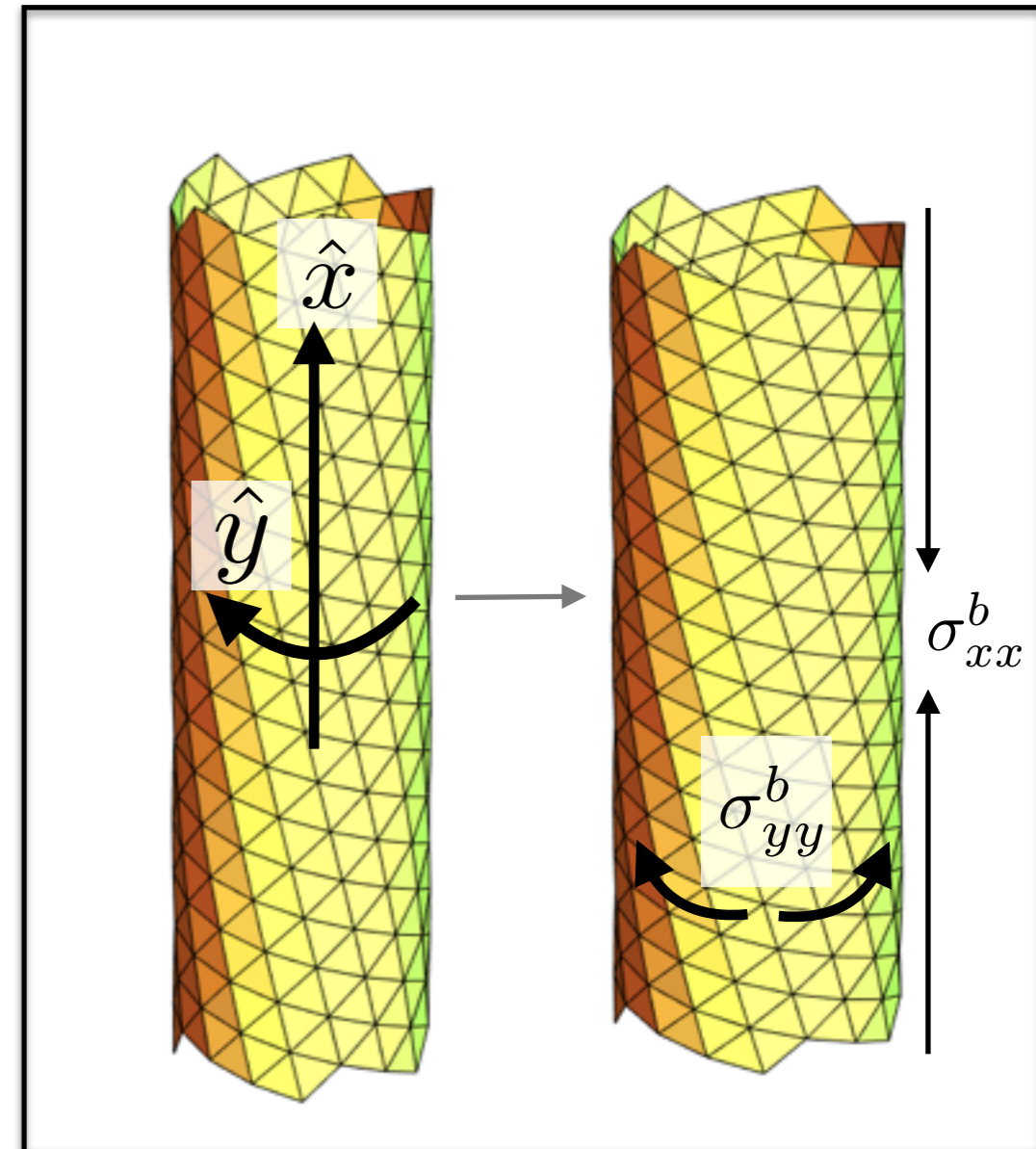
$$\sigma^b = \begin{pmatrix} \sigma_{xx}^b & \sigma_{xy}^b \\ \sigma_{xy}^b & \sigma_{yy}^b \end{pmatrix} = \frac{1}{2}Y\gamma^{-1} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$E_b = \frac{1}{2}\kappa \int d\mathbf{x}H^2 \rightarrow - \int d\mathbf{x}\sigma_{ij}^b u_{ij}$$

- Therefore, the *effective* critical tensile stress contains a simple “curvature offset”,

$$\begin{aligned} (\sigma_{xx} - \sigma_{yy})^{\dagger\text{eff}} &= (\sigma_{xx} - \sigma_{yy})^{\dagger} + (\sigma_{xx}^b - \sigma_{yy}^b) \\ &= (\sigma_{xx} - \sigma_{yy})^{\dagger} - Y\gamma^{-1} \end{aligned}$$

$$\text{Föppl-van Kármán number } \gamma \equiv \frac{Y R^2}{\kappa} \gg 1$$



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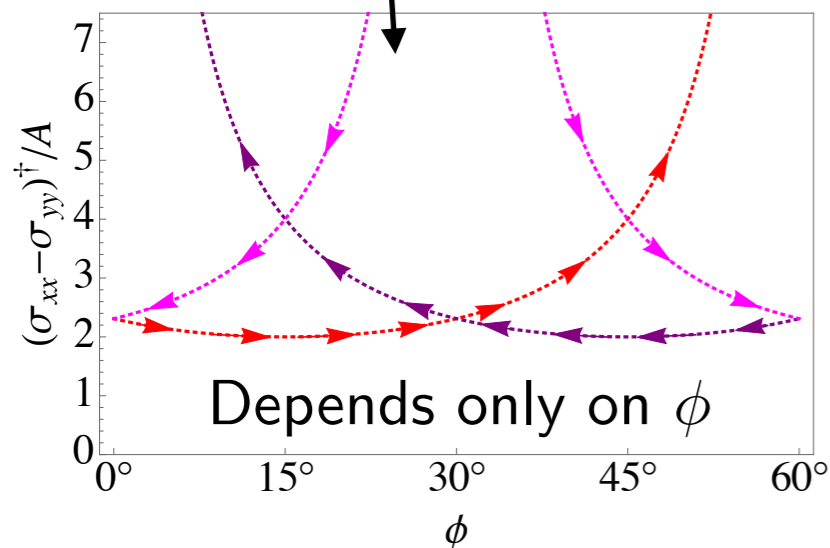
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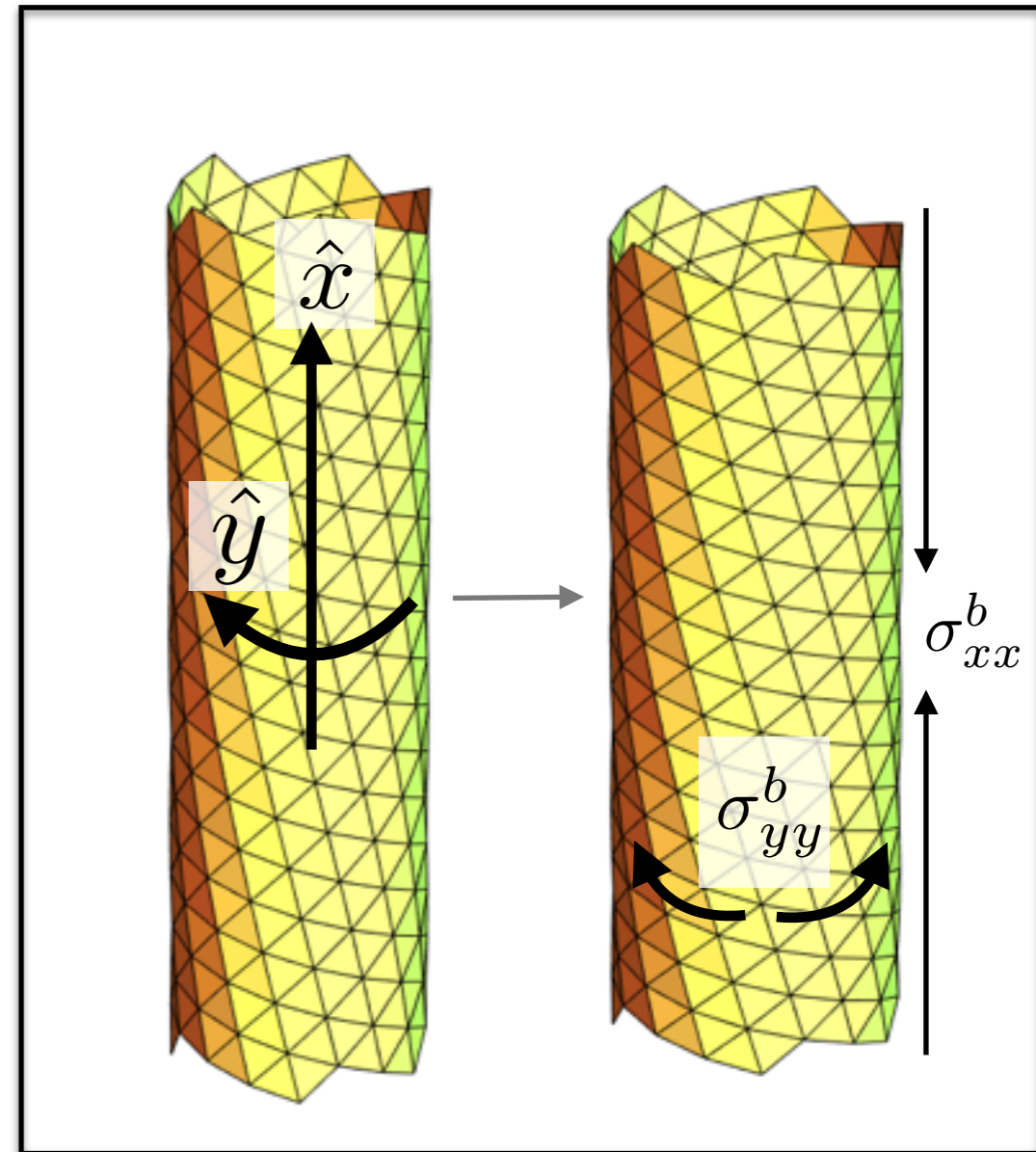
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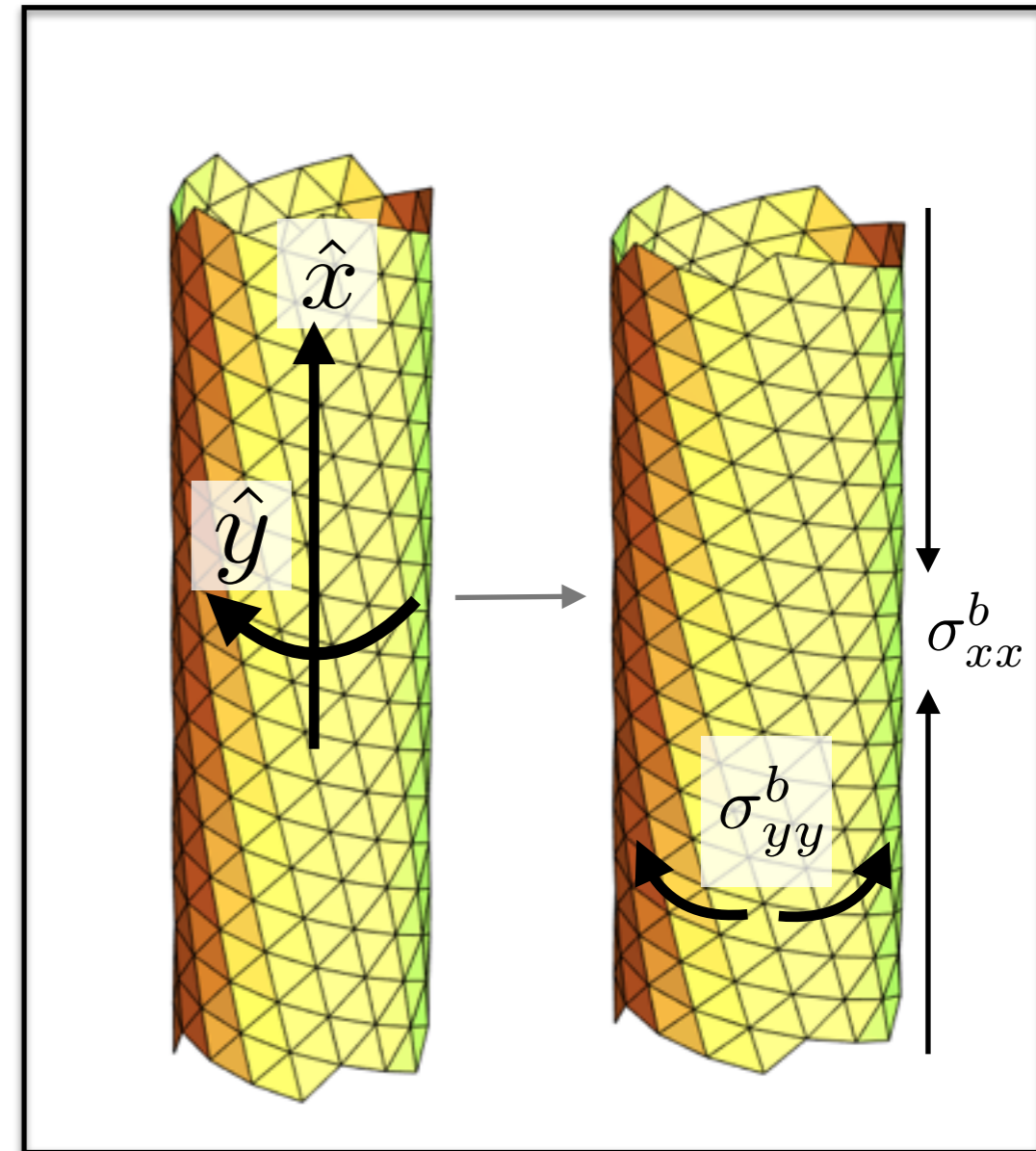
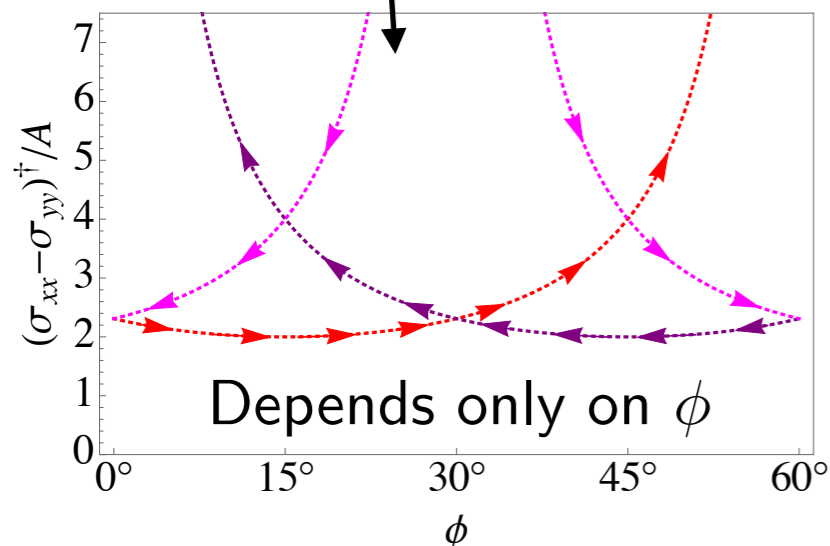
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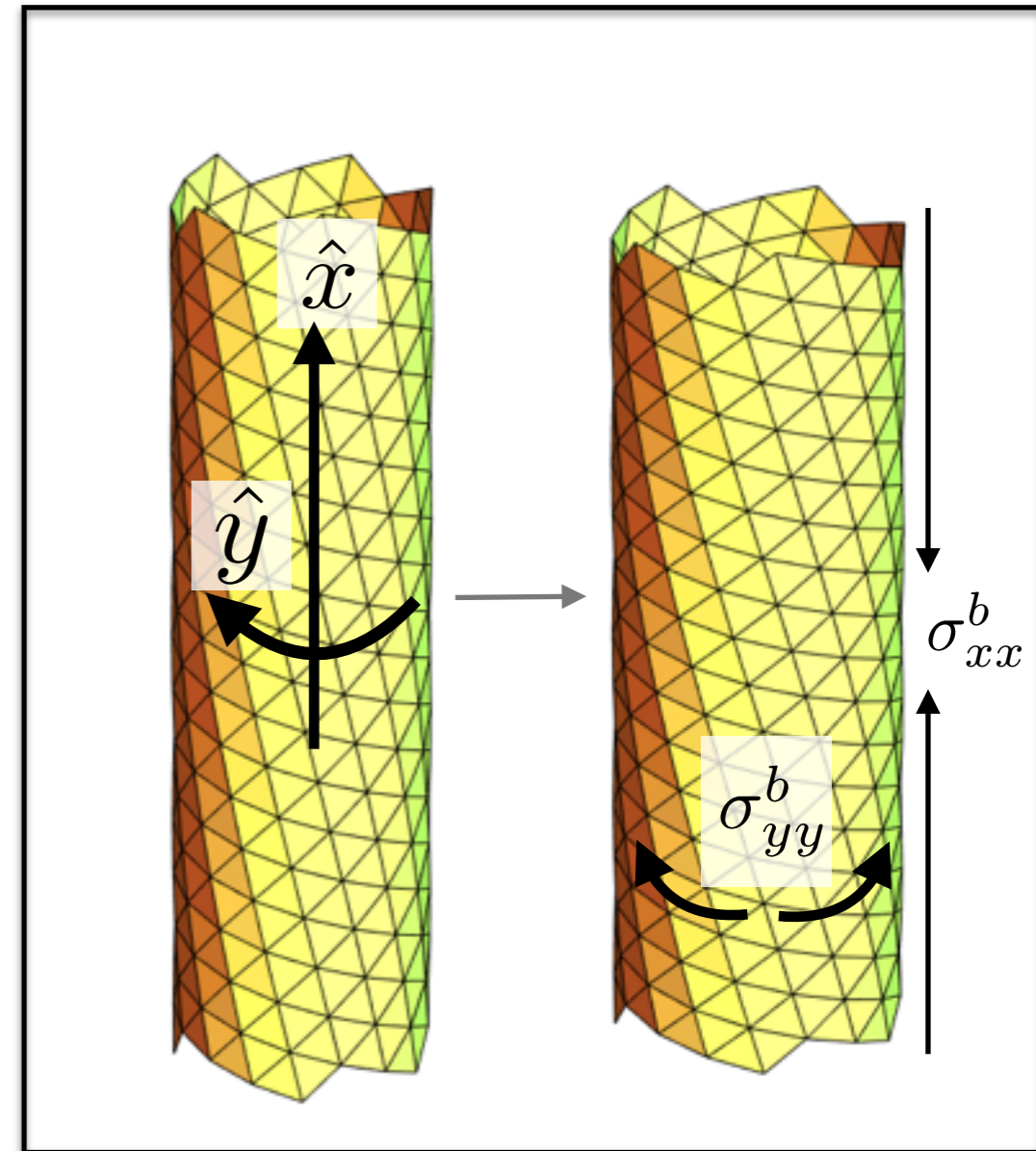
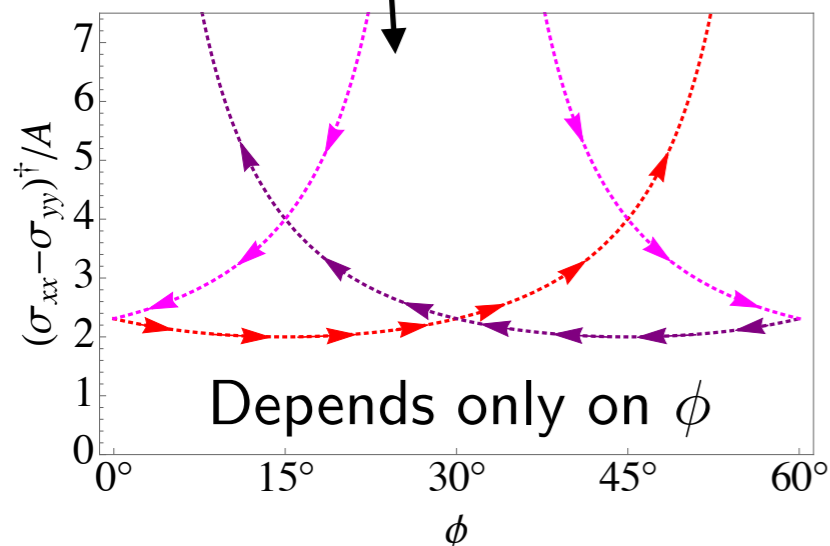
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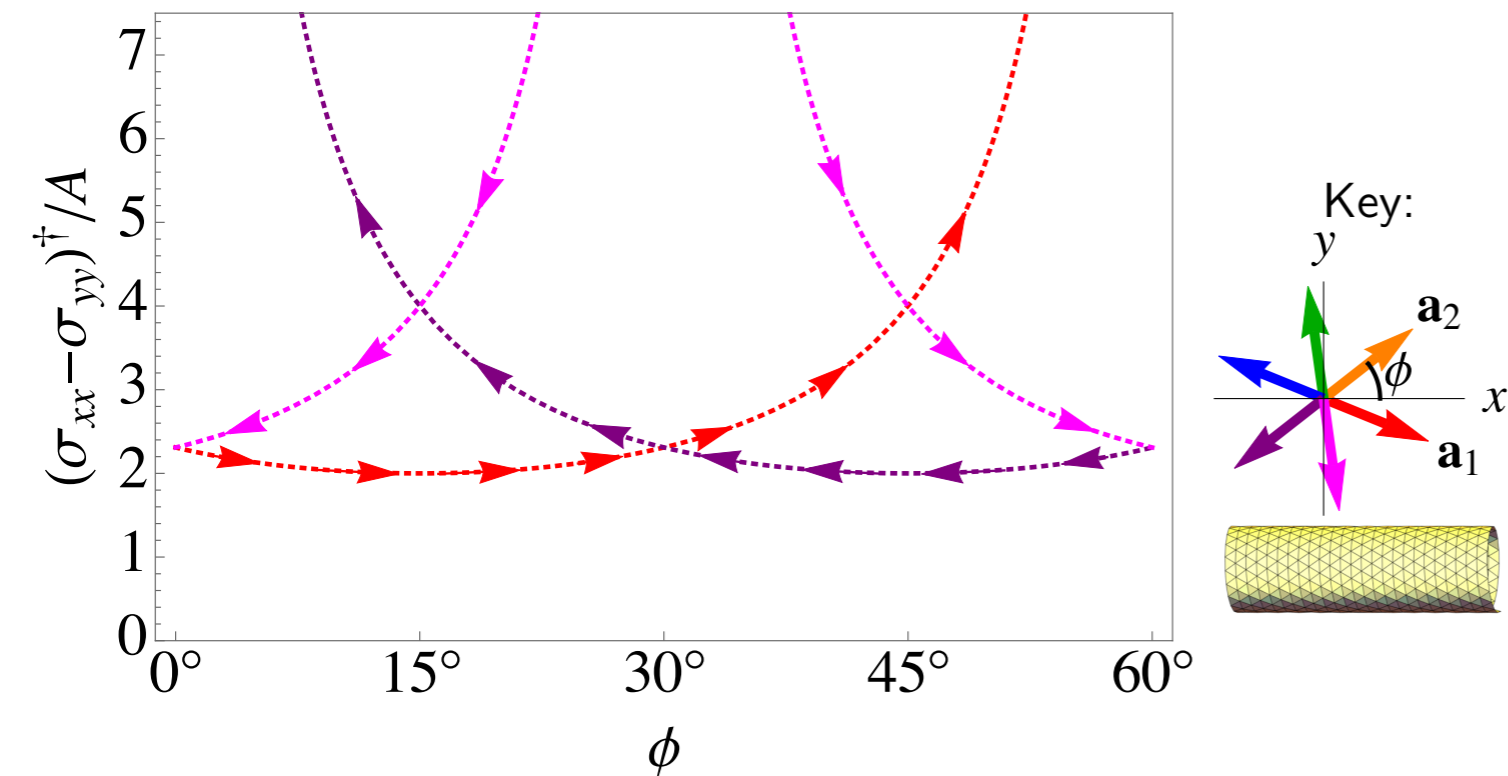
- Bending energy opposes plastic deformations that decrease R .
- Larger $\kappa \Rightarrow$ larger $\gamma^{-1} \Rightarrow$ greater stress required to unbind dislocations.

Bending energy may make very narrow tubes unstable

- $(\sigma_{xx} - \sigma_{yy})^{\dagger \text{eff}} = (\sigma_{xx} - \sigma_{yy})^{\dagger} - Y\gamma^{-1}$
- What happens when $Y\gamma^{-1} > \sigma_c \approx 2A$?
- Then, with zero external stress, it is energetically favorable to unbind dislocation pairs that *widen* the tube.
- Tubes are unstable if

$$R < \boxed{R_c = \sqrt{\kappa/\sigma_c(\phi)}}$$

- (Need $\tilde{\kappa} \equiv \kappa Y/a^2 \gtrsim 0.2$ in order for $R < R_c$ to be geometrically possible.)

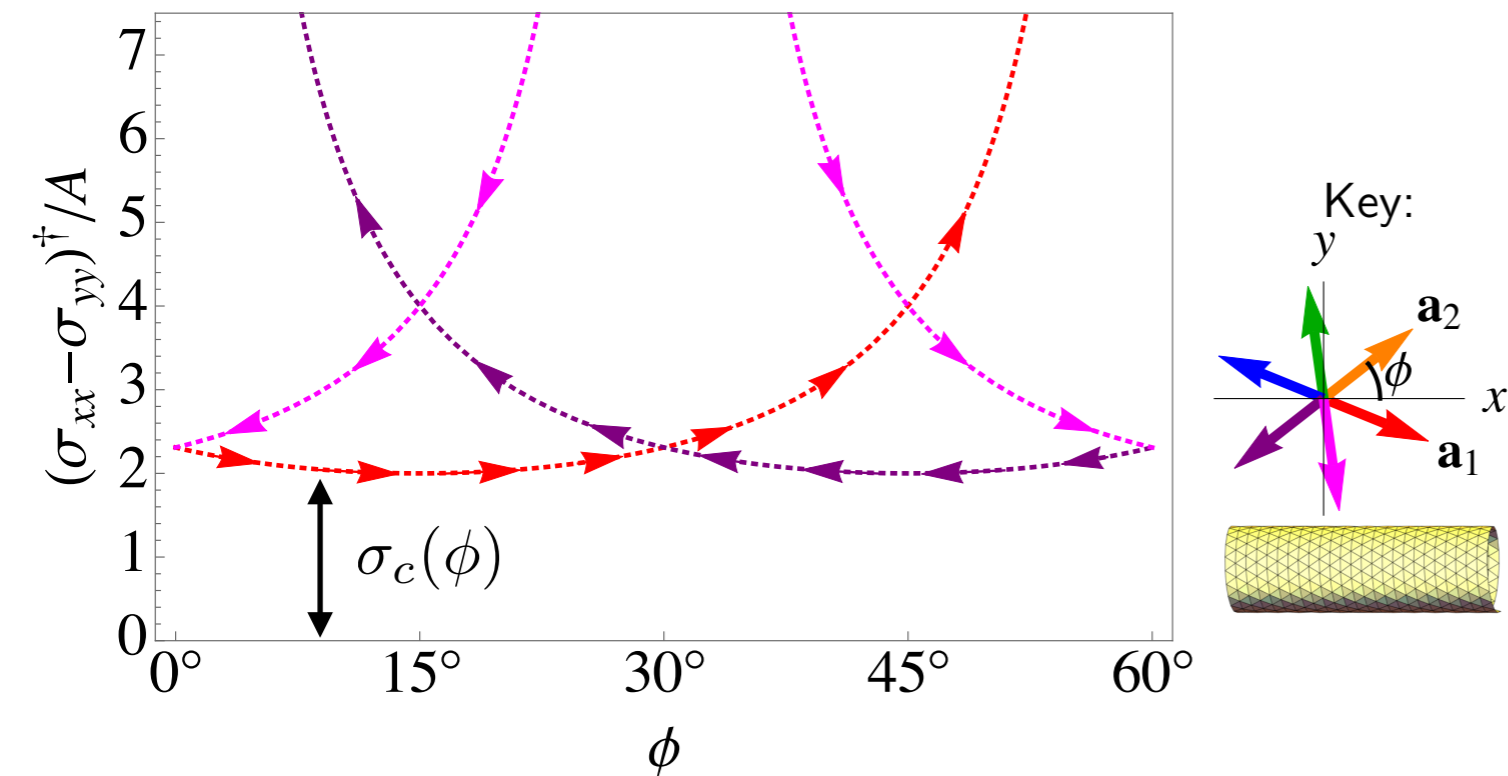


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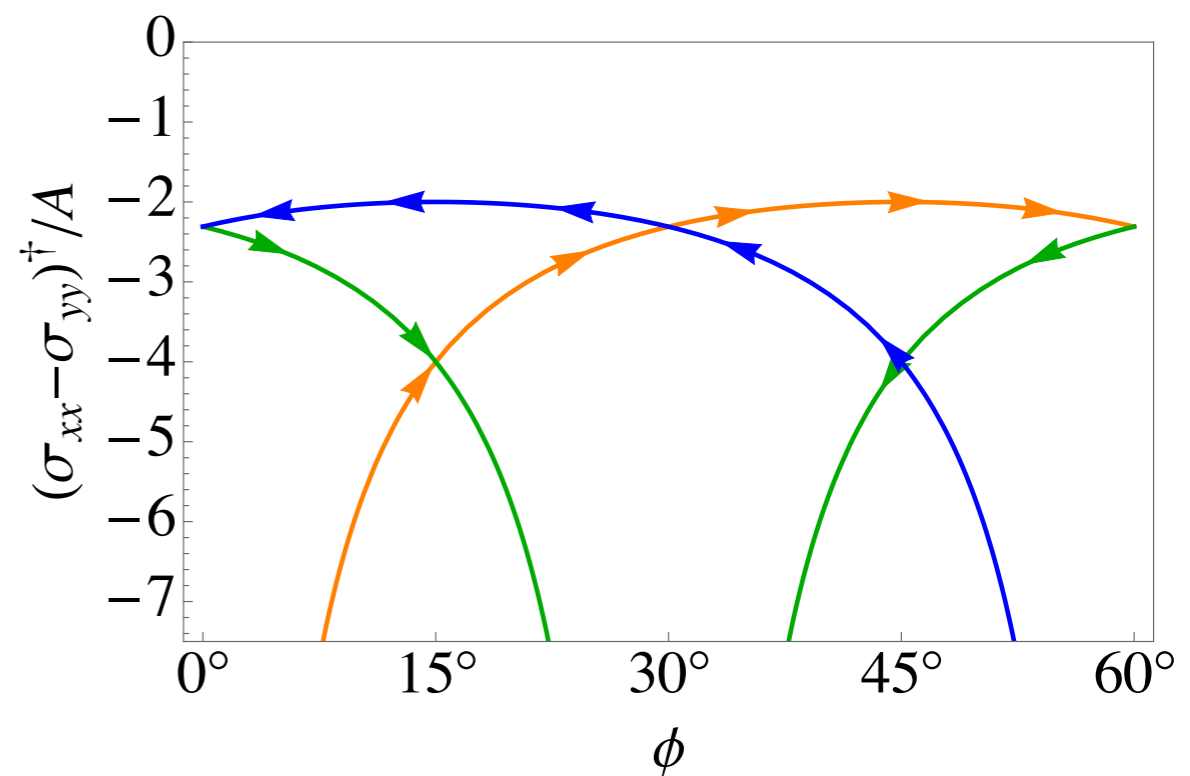
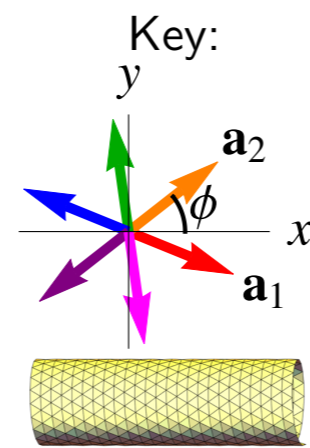
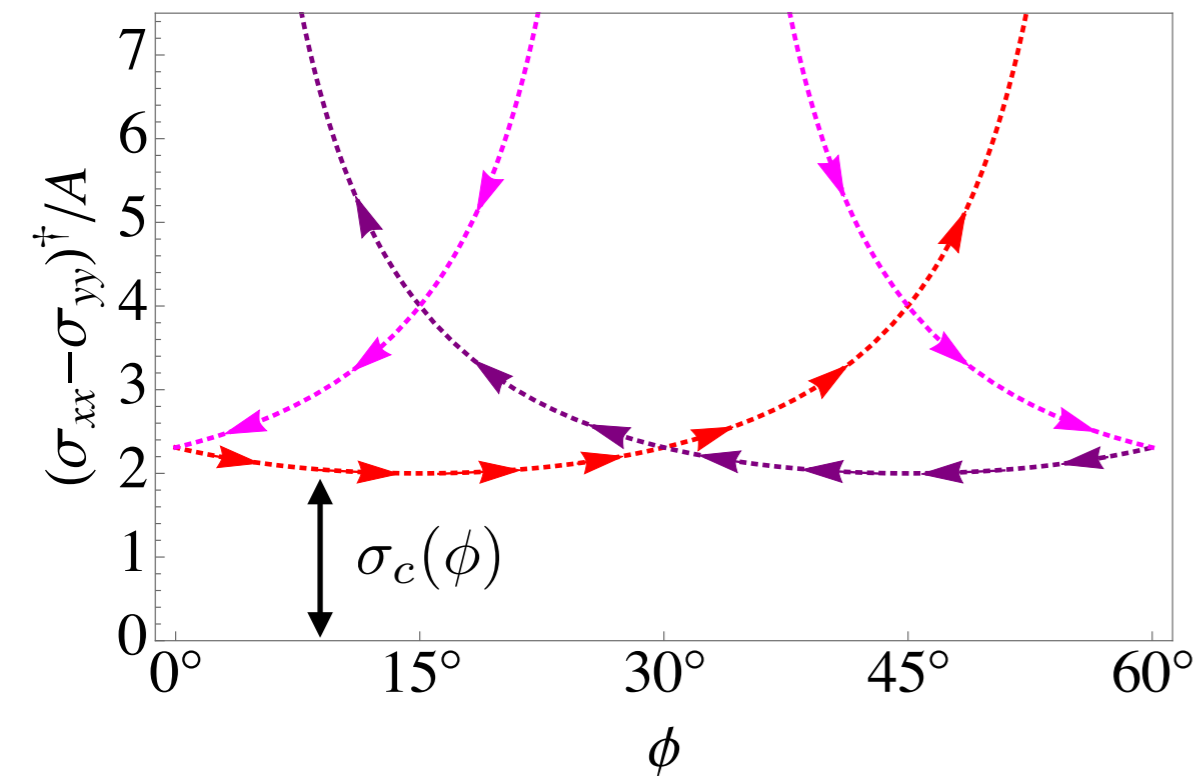


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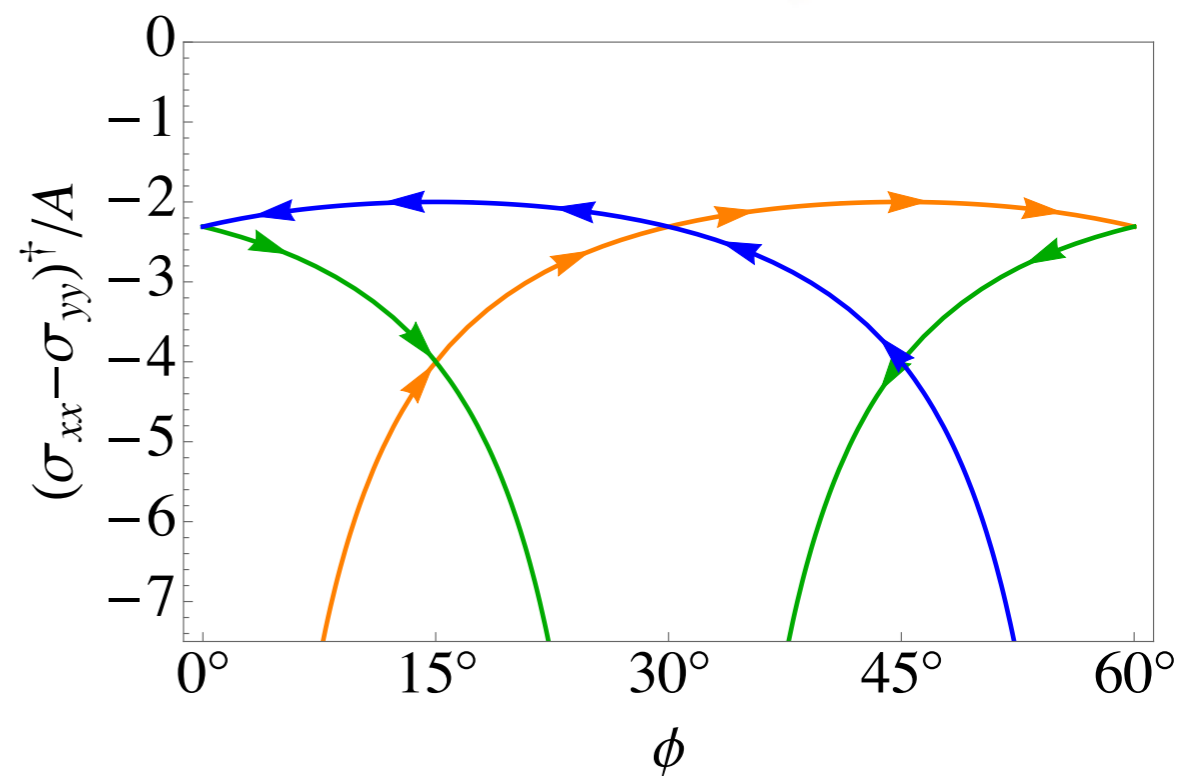
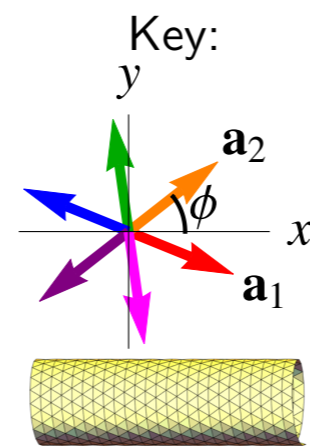
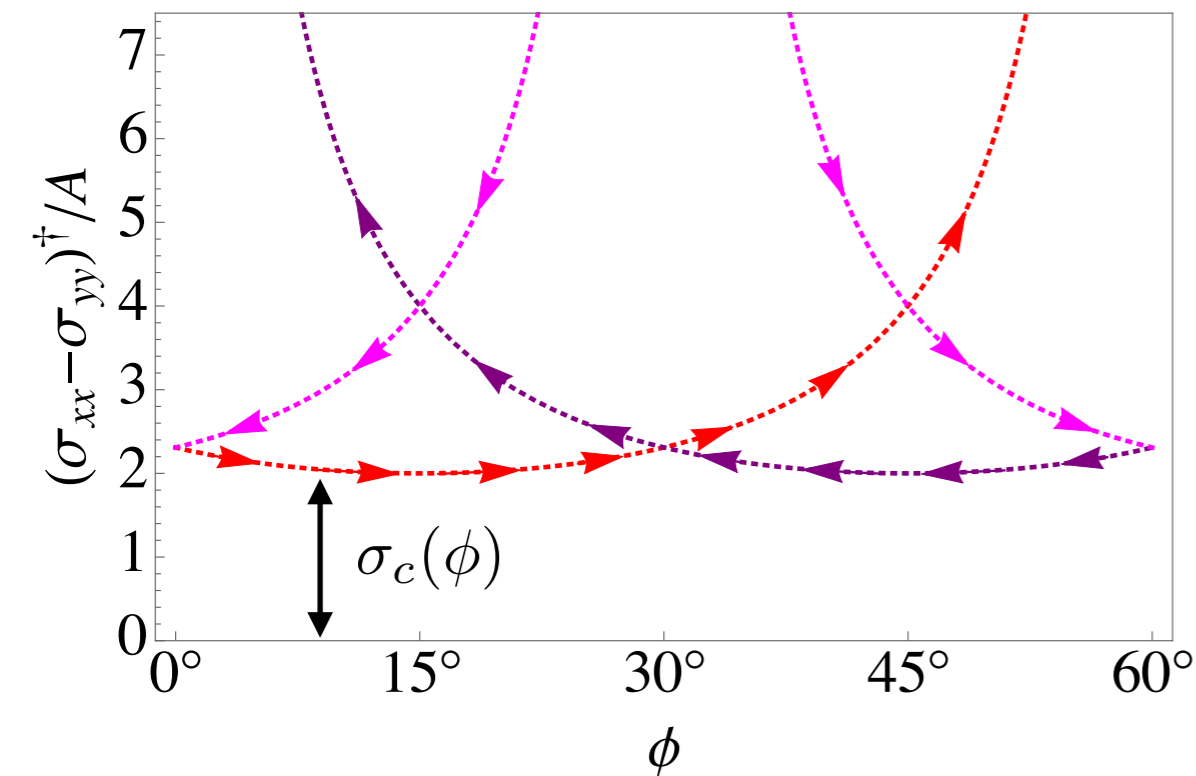
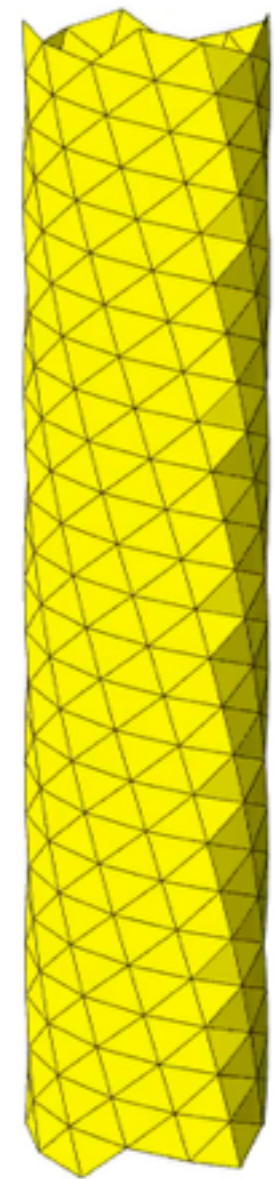


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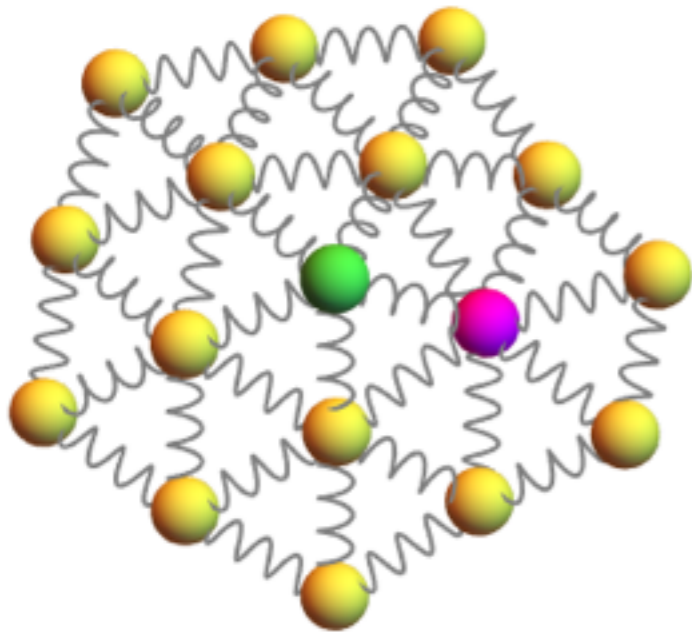
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Plastic deformation of tubular crystals

- Background: Phyllotactic geometry of tubular crystals
- Mechanics of plastic deformation: Analytic predictions
- Numerical modeling
- Necks in tubes: Radius profiles near dislocations

Numerical modeling of tubular crystals



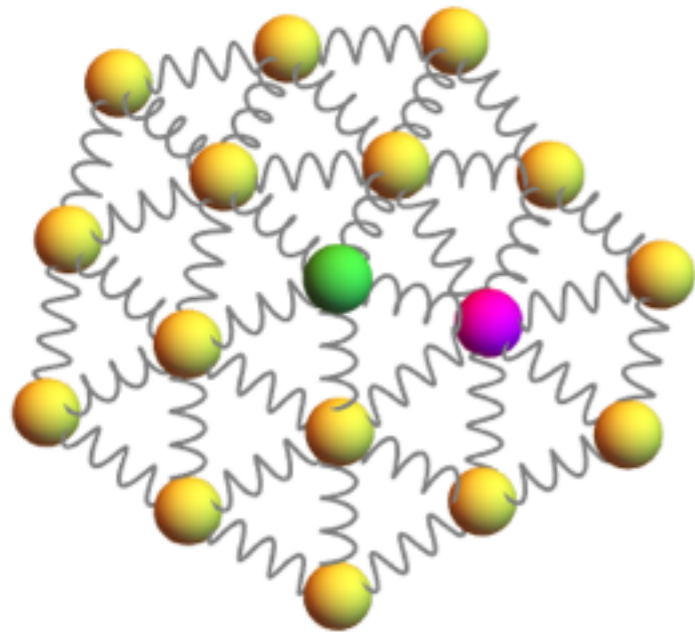
- “Ball and spring model”: Nodes connected by harmonic springs*
 - Rest length $a = 1$
 - Spring constant $k = (\sqrt{3}/2)Y$
- Bending energy penalizes mean curvature when neighboring nodes are not coplanar**.
 - Bending rigidity $\tilde{\kappa} = \kappa Y/a^2$

* Seung and Nelson, Phys. Rev. A 38:1005 (1988)

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- Periodic boundary conditions along the cylinder axis:
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Numerical modeling of tubular crystals

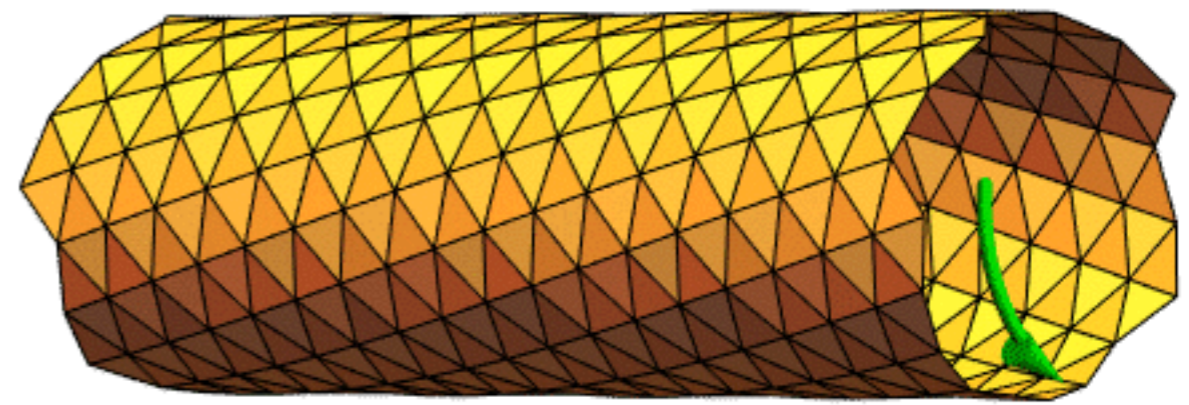
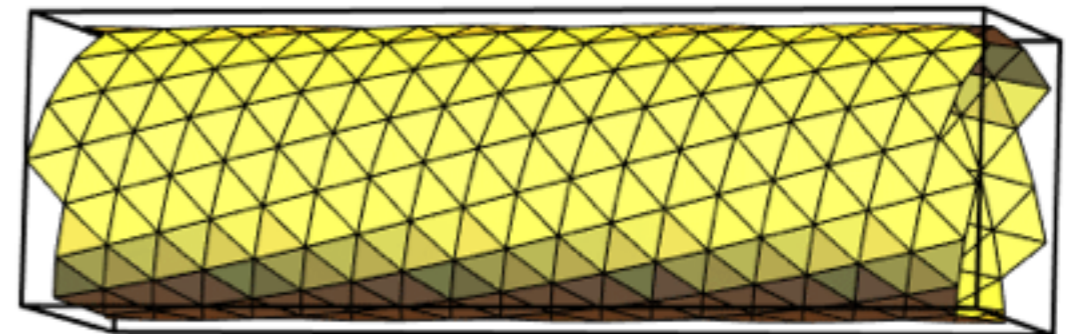


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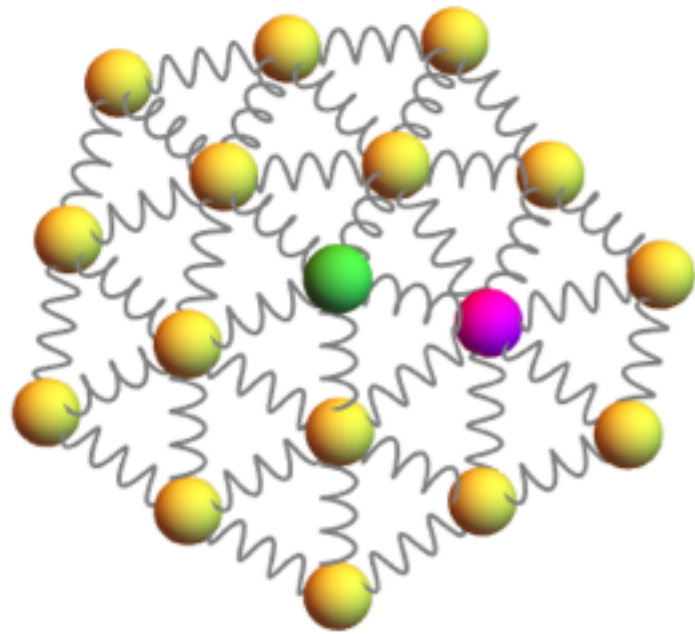
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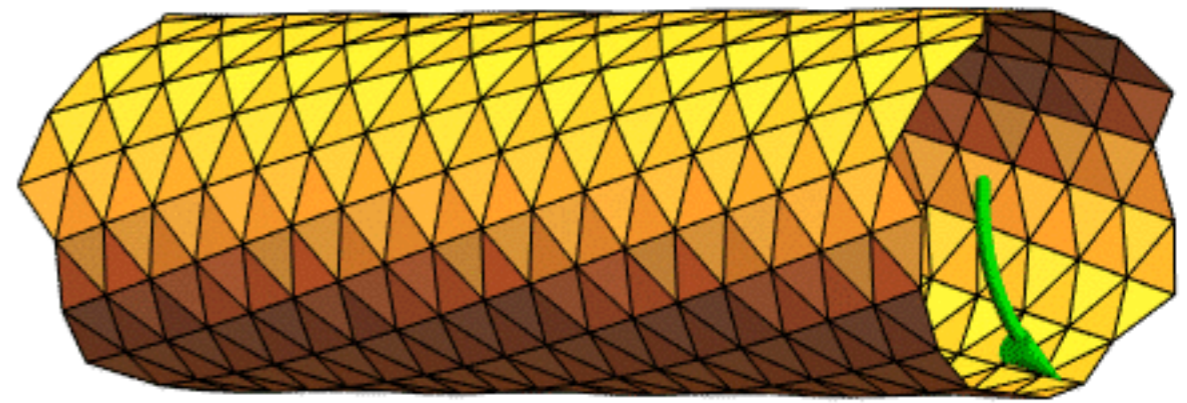
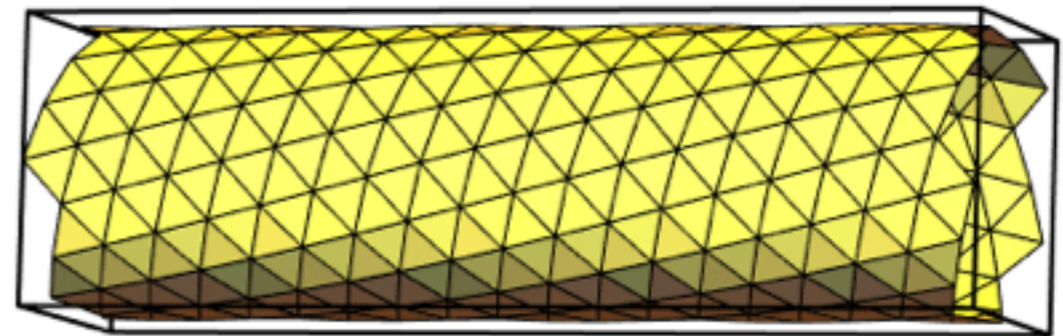


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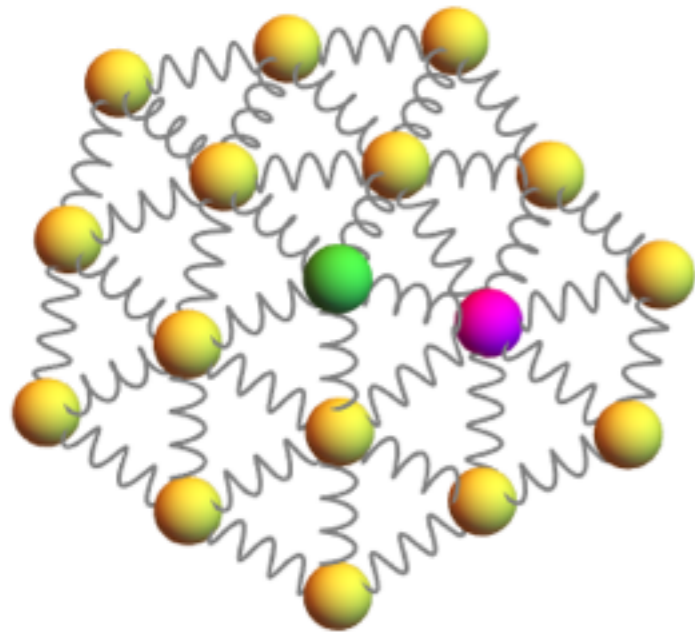
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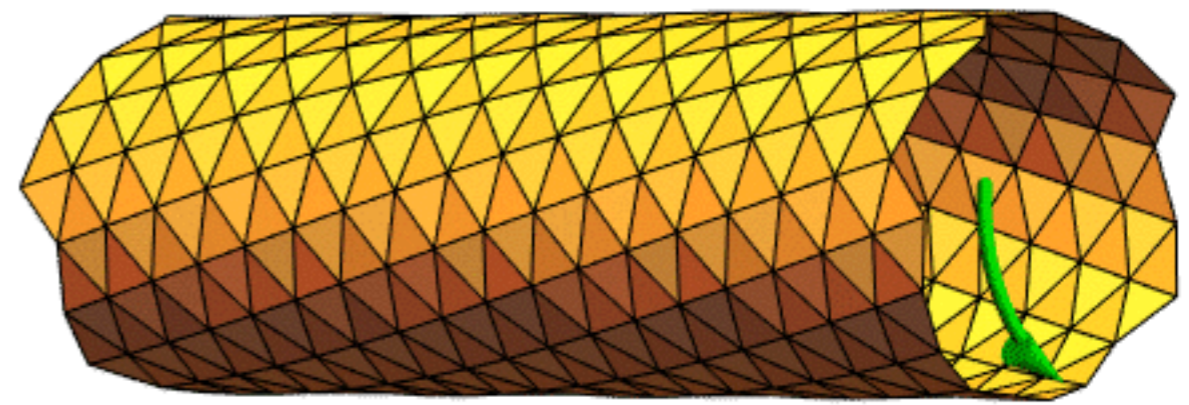
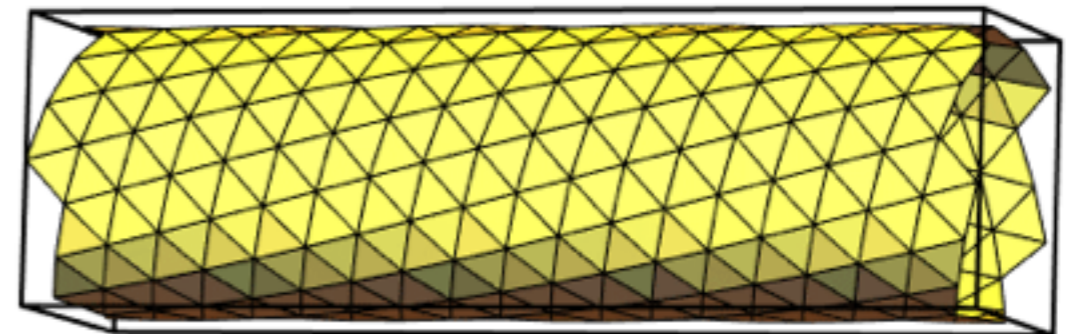


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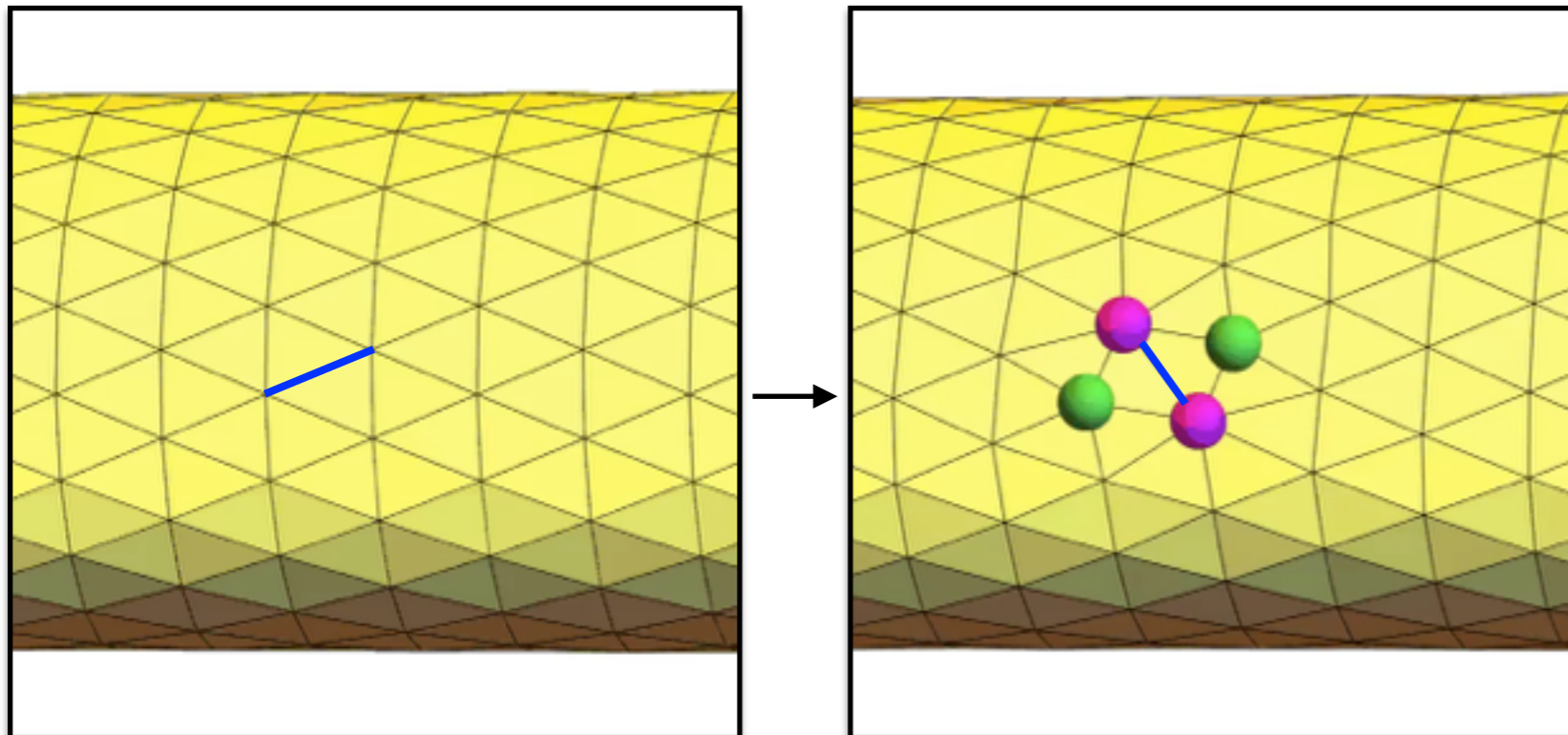
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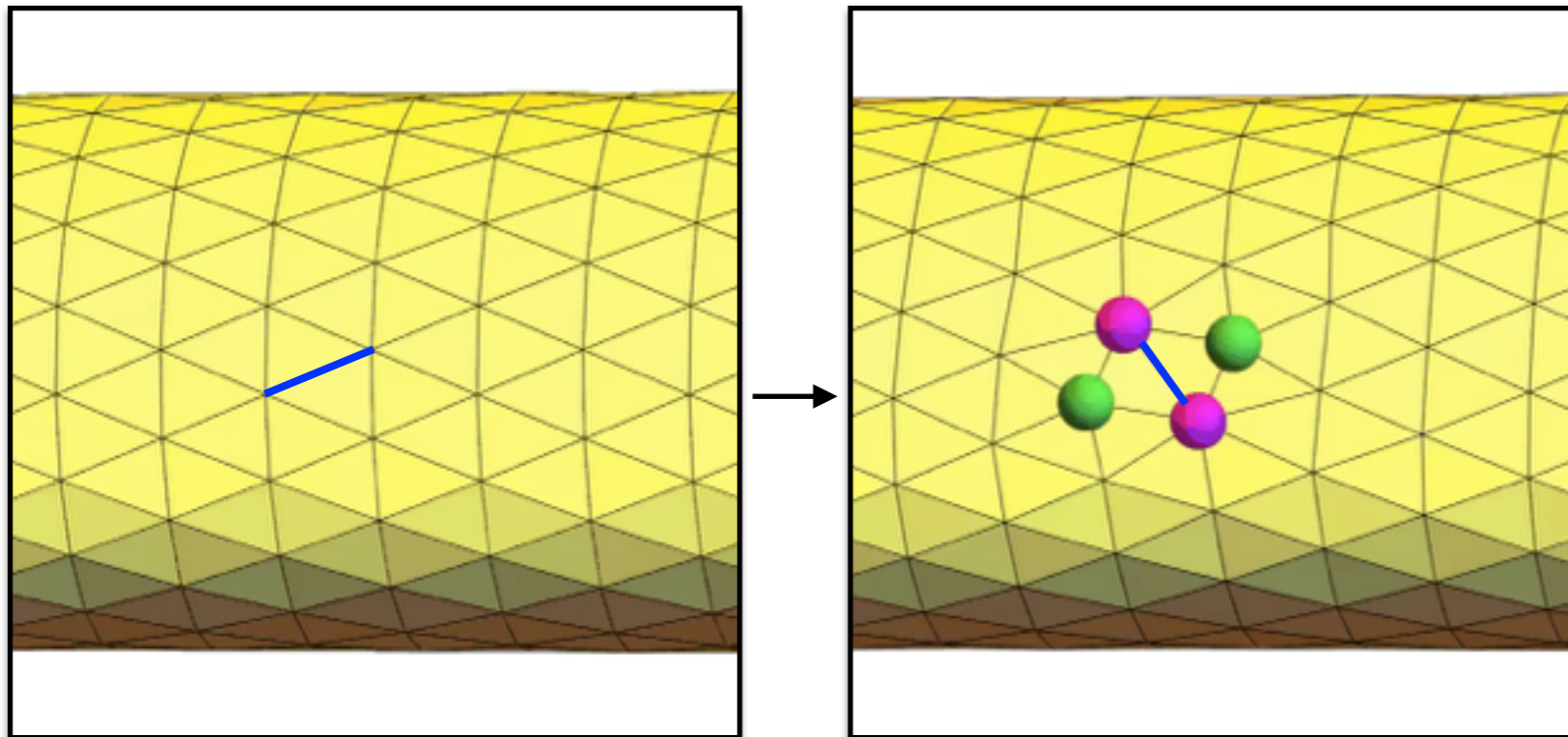
Numerical modeling of tubular crystals

- Dislocation glide via bond flips (plastic; slow timescale)
- Node positions update to minimize total energy (elastic; fast timescale)
- Glide move accepted only if it lowers the energy



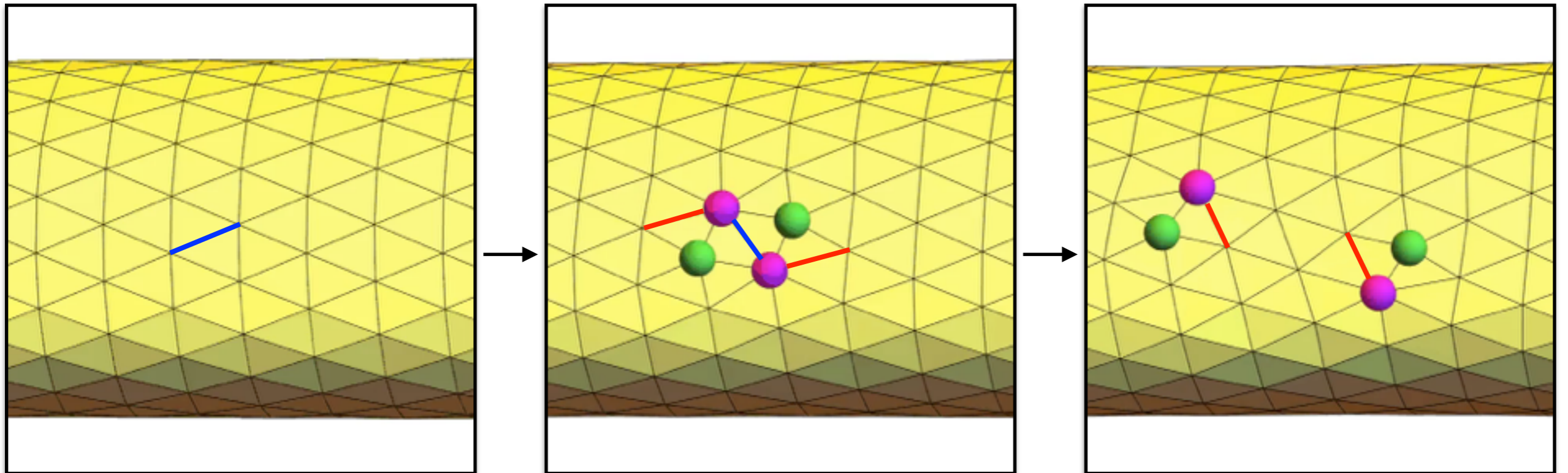
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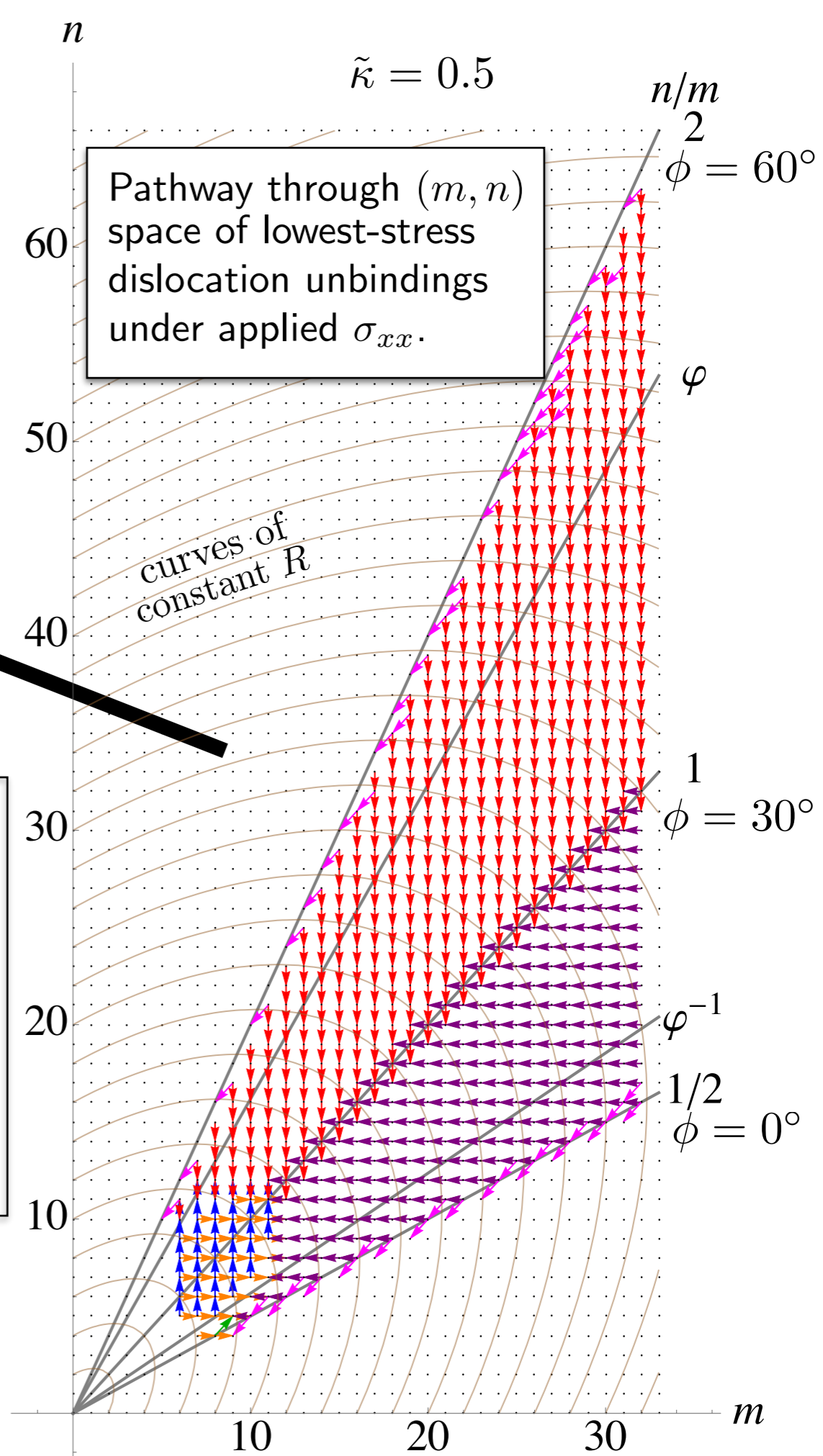
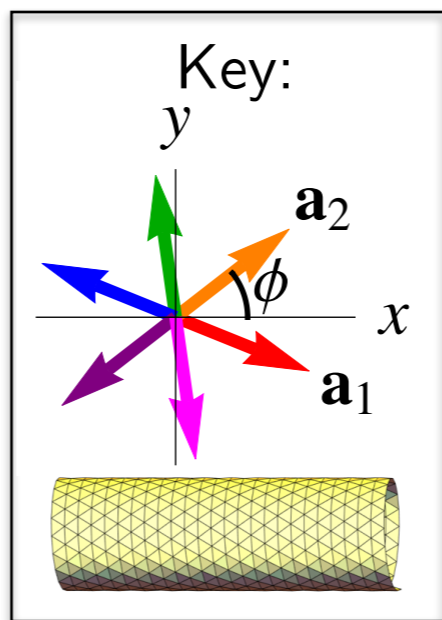
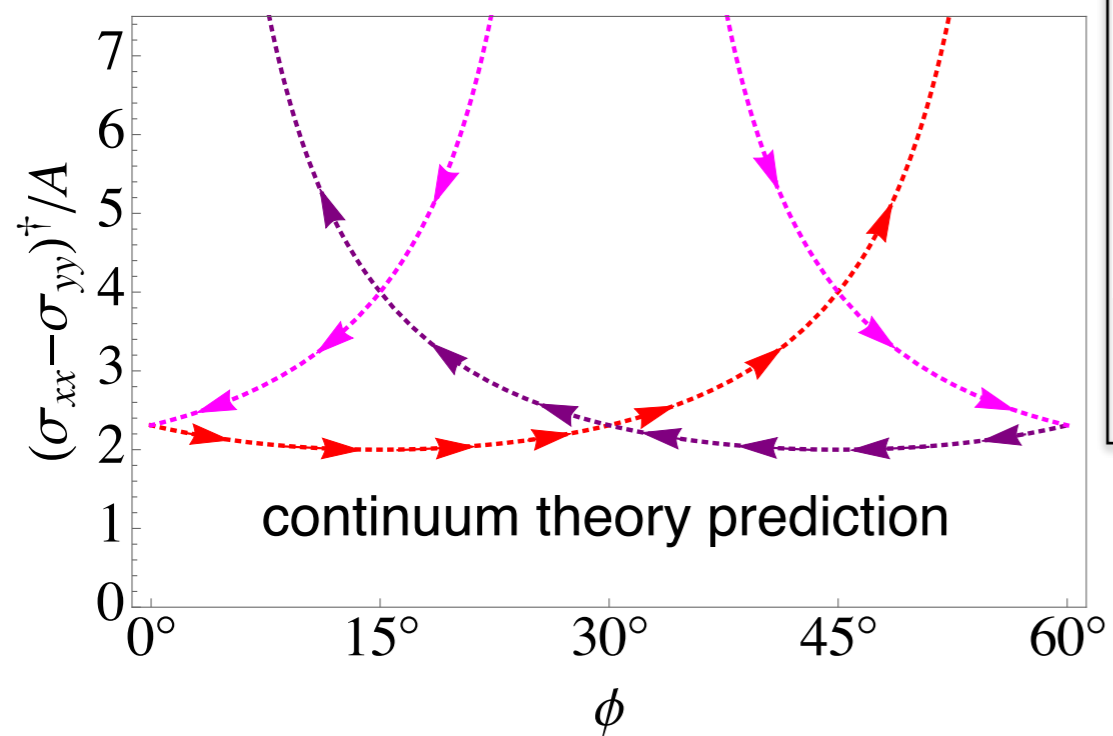
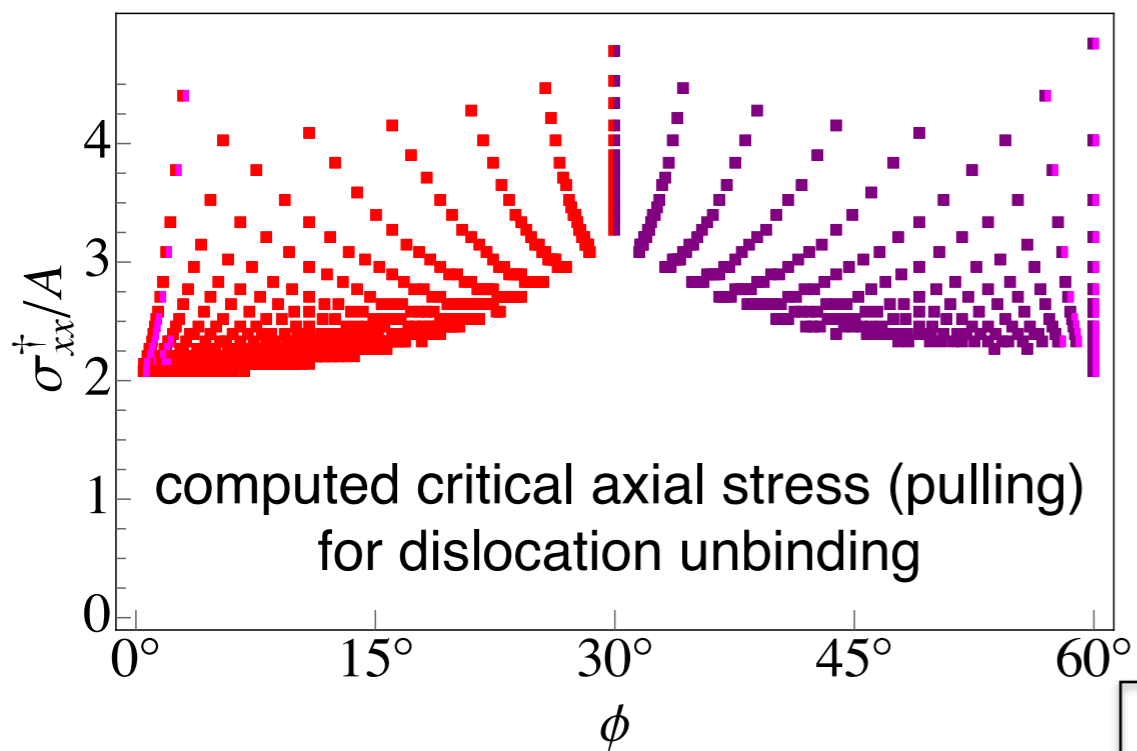


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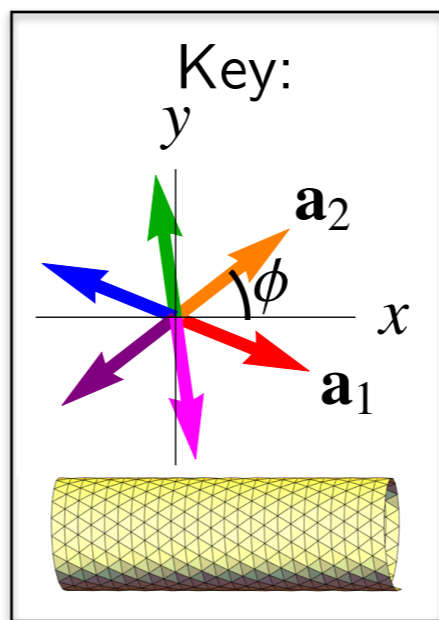
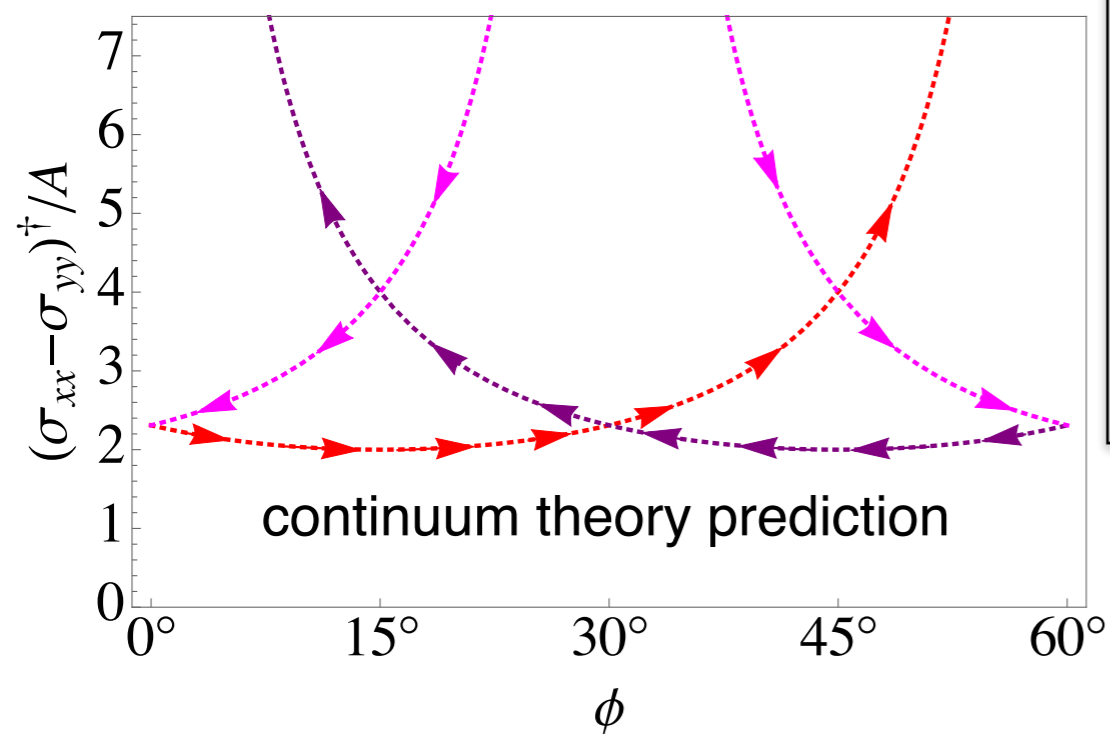
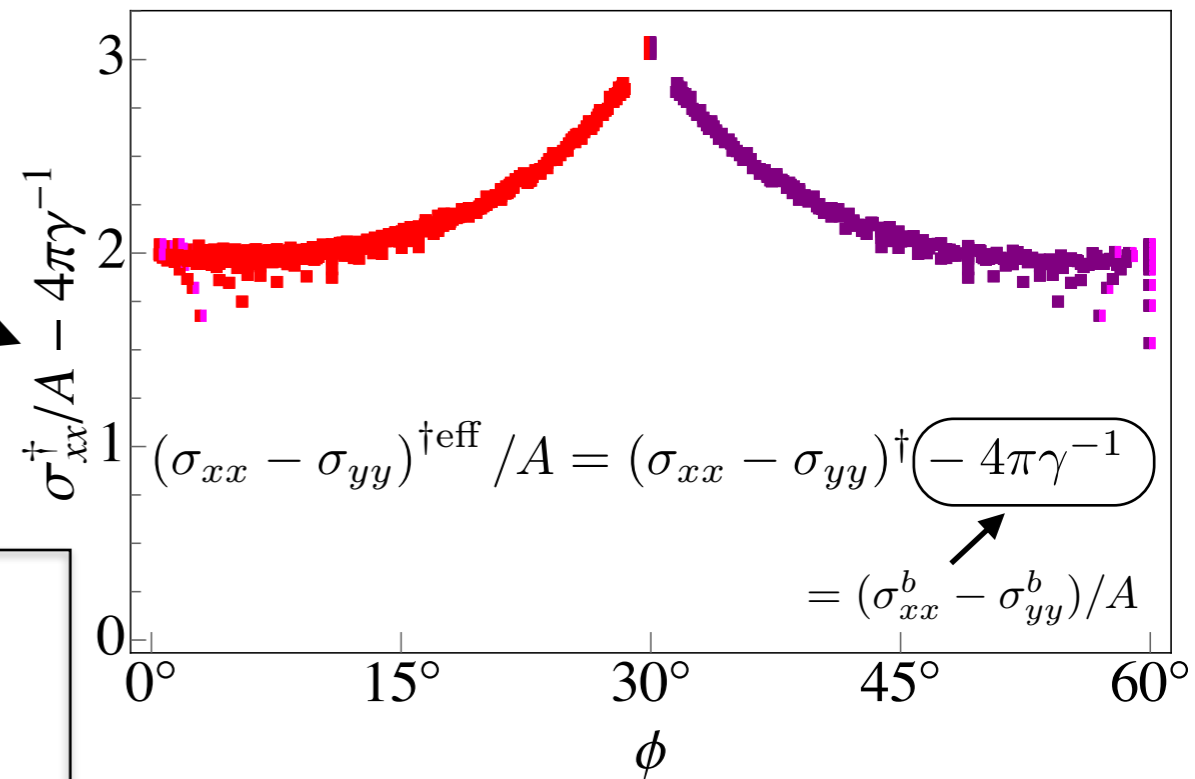
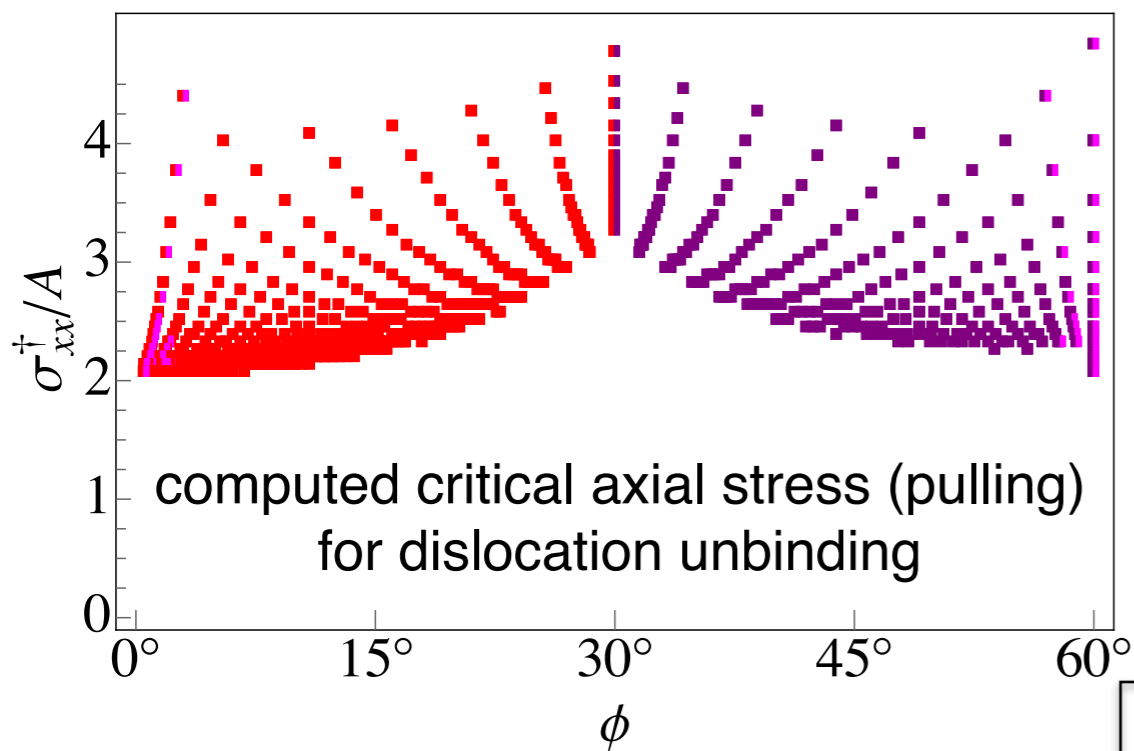
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Tubes under axial tension: Numerical results



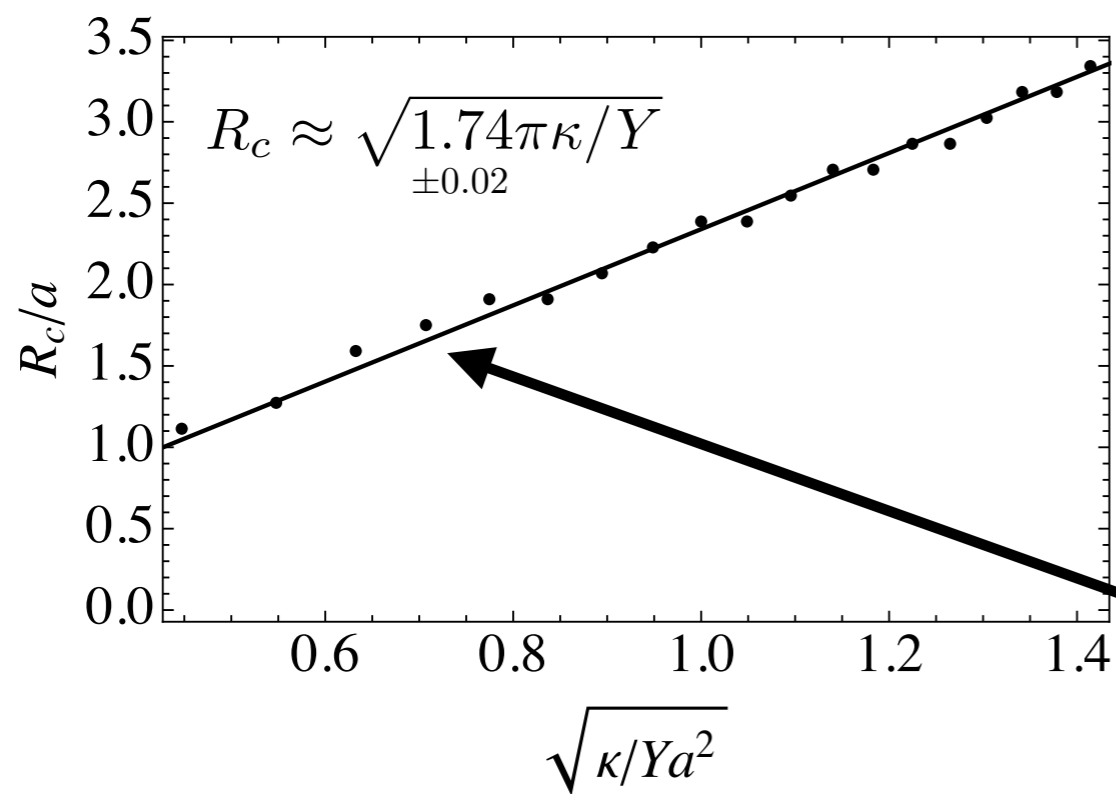
Tubes under axial tension: Numerical results



Computed σ_{xx}^\dagger collapses to R -independent curve $\sigma_{xx}^{\dagger\text{eff}}$ when we offset the applied stress by the bending energy's effective stress.

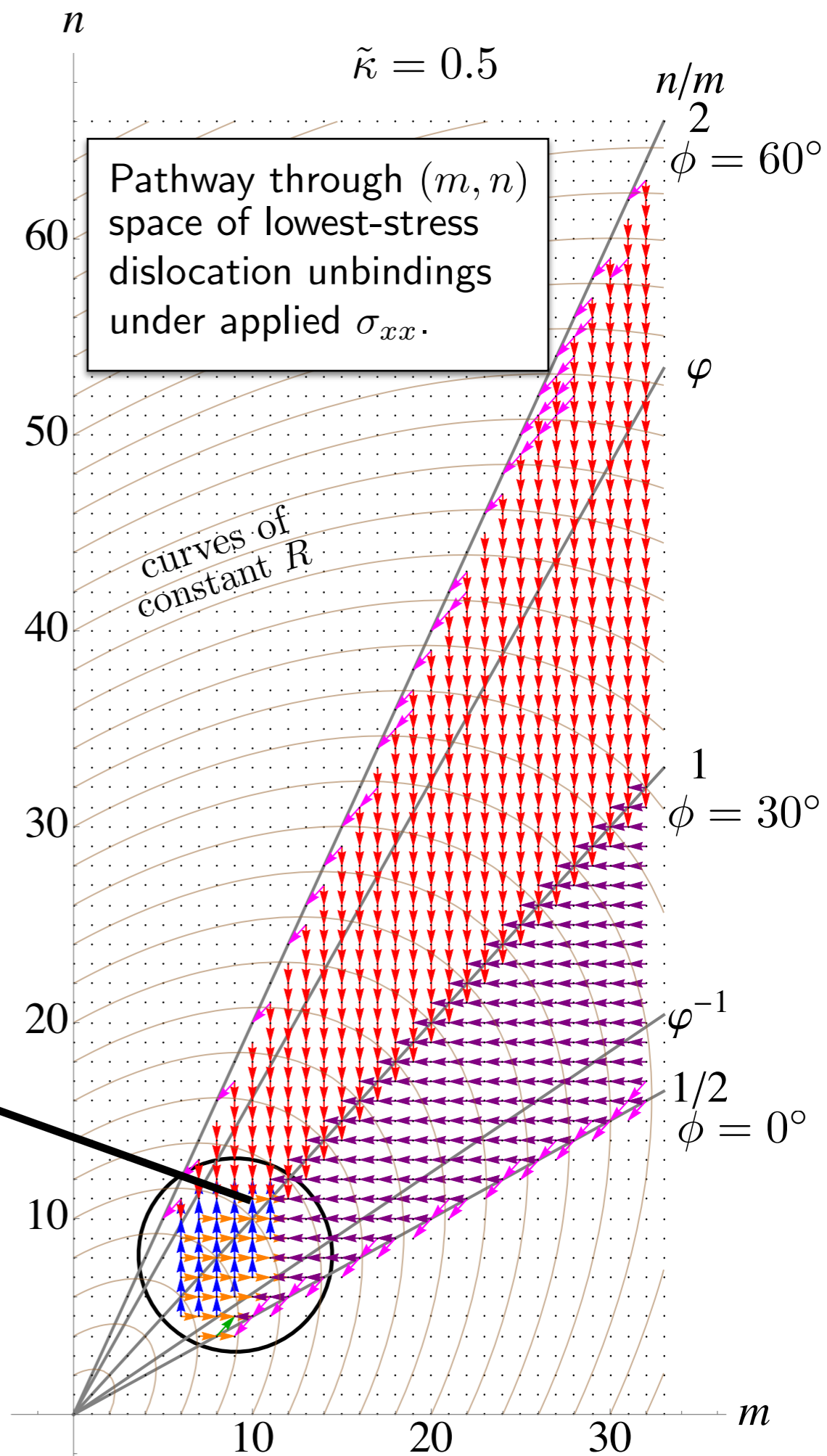
Tubes under axial tension: Numerical results

The bending energy makes narrow tubes with $R < R_c$ unstable to spontaneous dislocation unbindings that widen the tube.



Continuum theory predicts

$$R_c = \sqrt{\kappa/\sigma_c} = \sqrt{\sqrt{3}\pi\kappa/Y} \approx \sqrt{1.73\pi\kappa/Y}$$

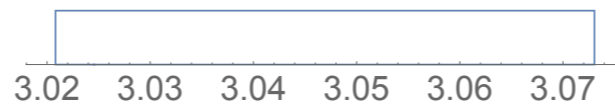
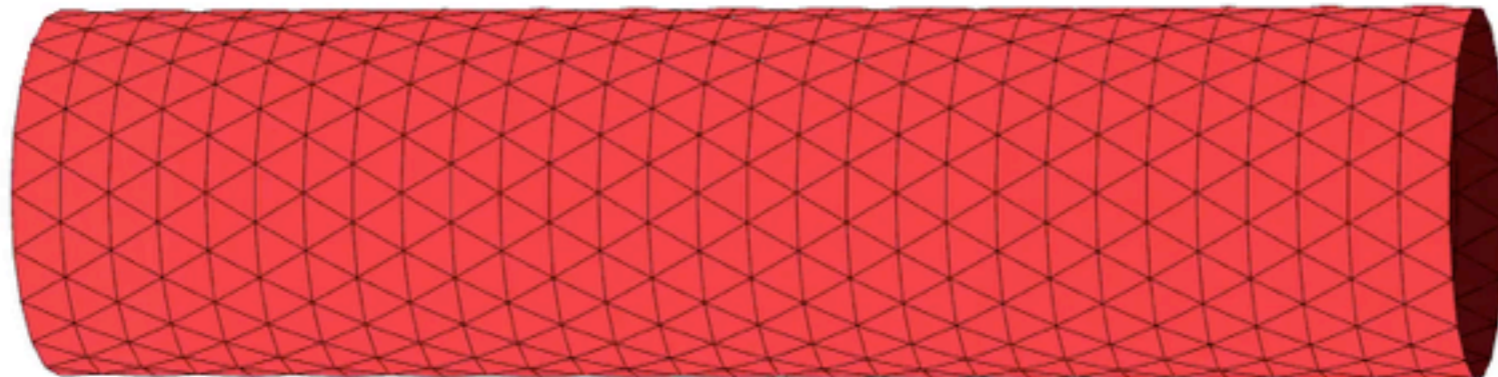
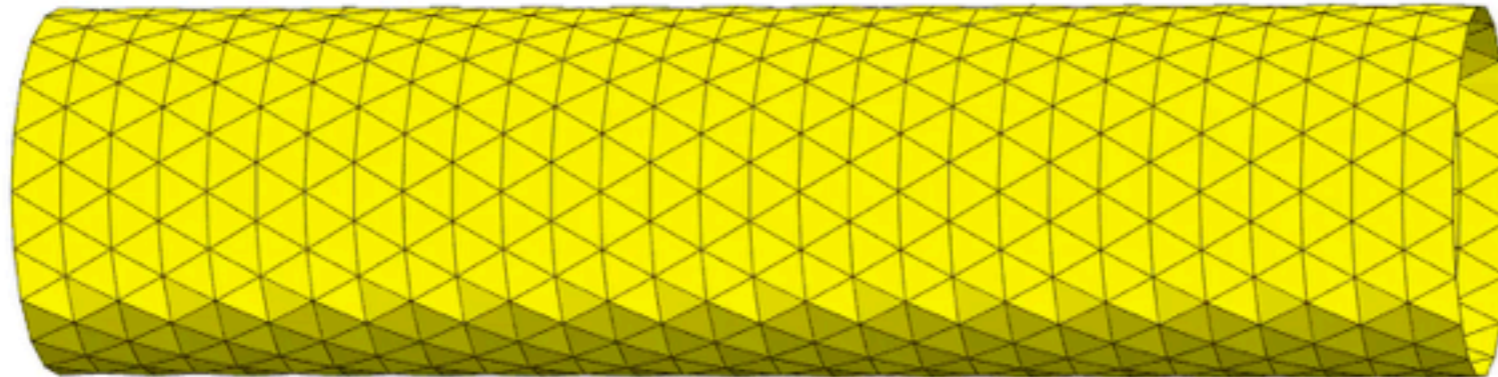


Plastic deformation of tubular crystals

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The shape of a tube containing dislocations

$$(20, 20) \rightarrow (20, 19)$$

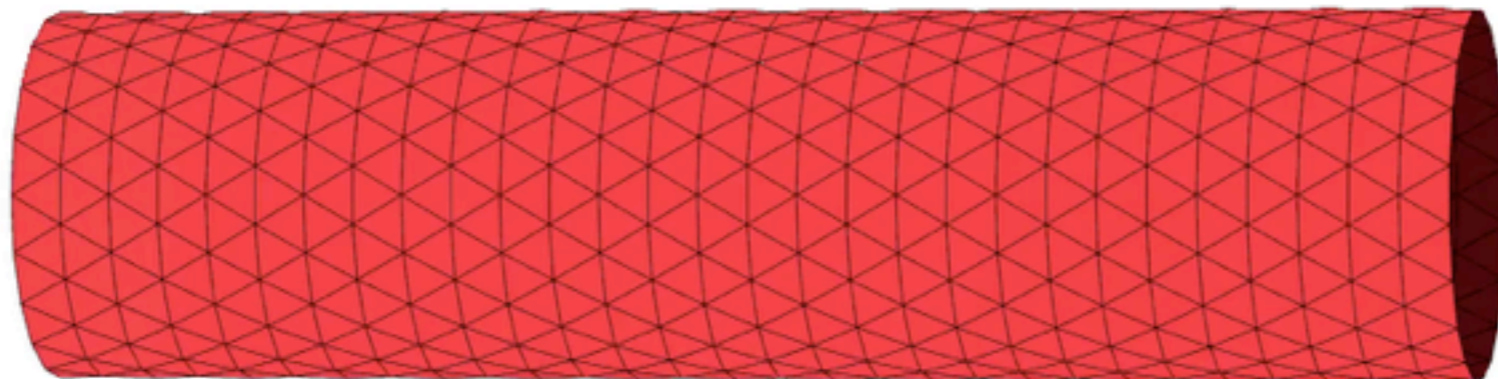
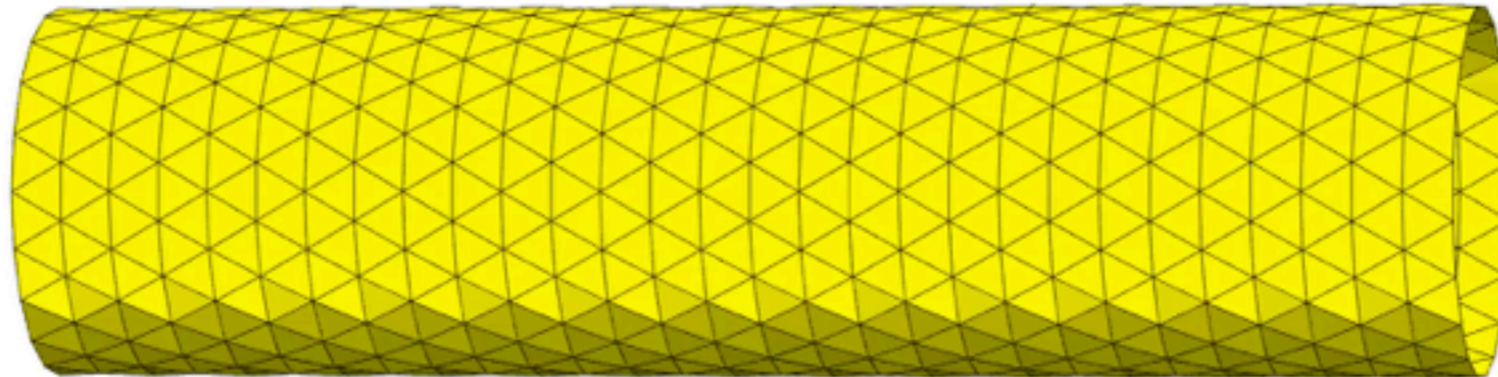


Radius/lattice spacing

Local radius $R(\mathbf{x})$ tracks dislocation motion

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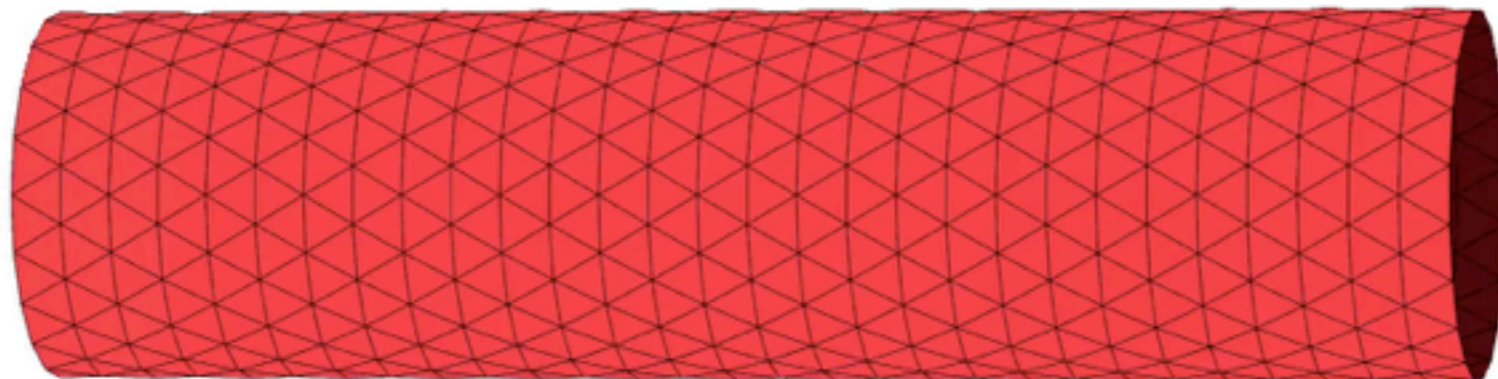
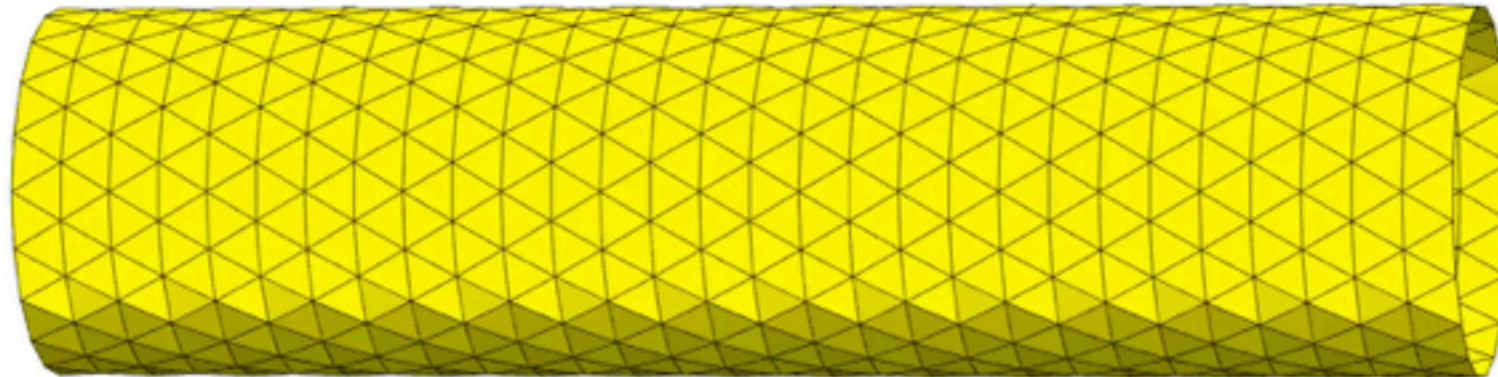


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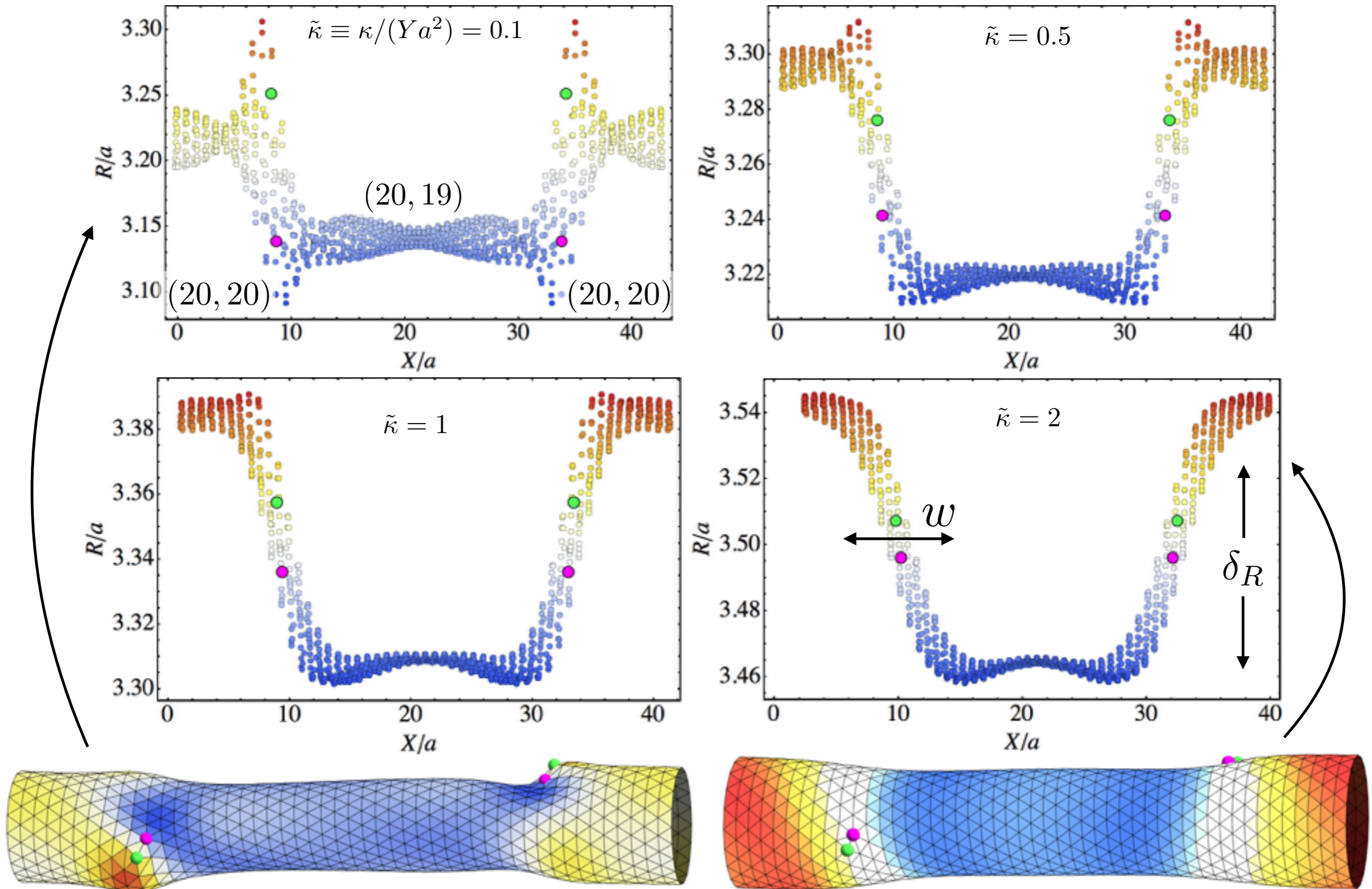
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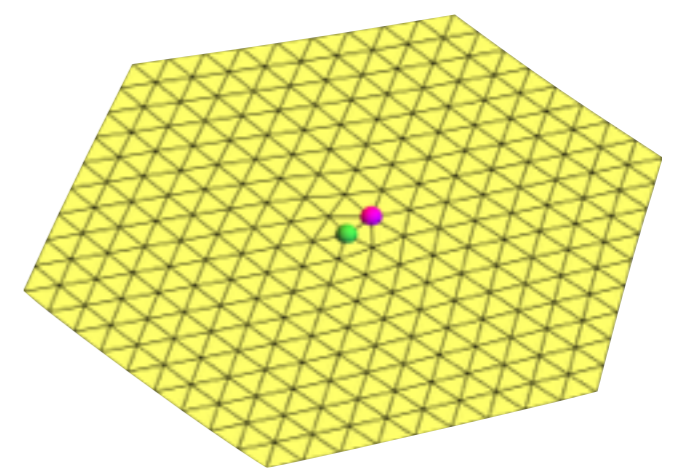
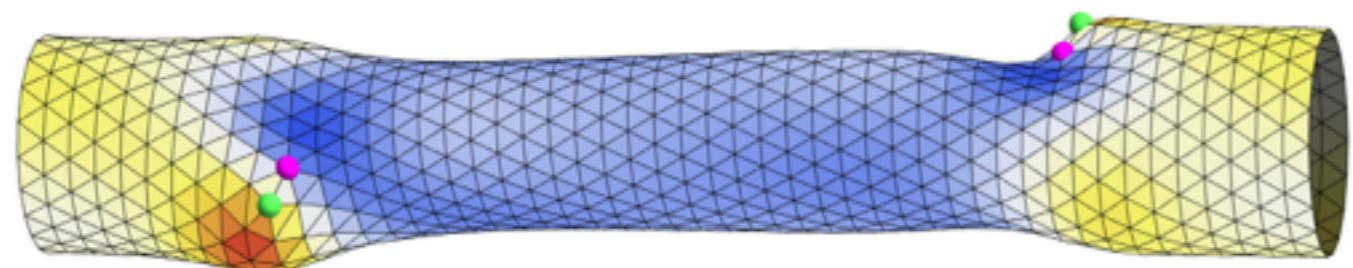
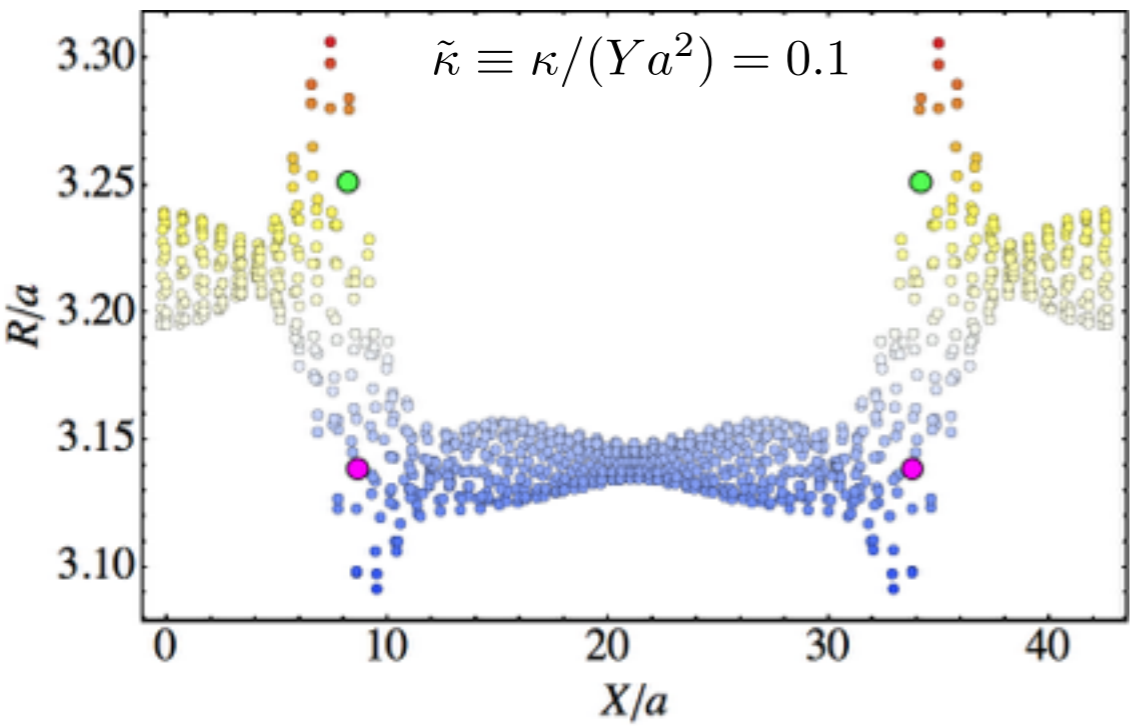
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The shape of a tube containing dislocations



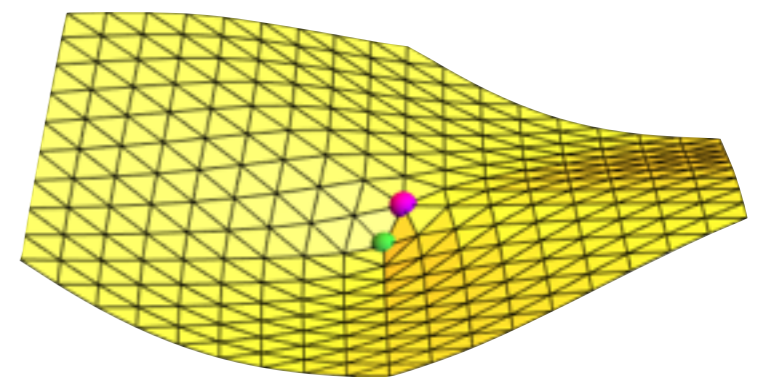
Buckling at small $\tilde{\kappa}$



$$\frac{R}{a\tilde{\kappa}} \approx 90$$

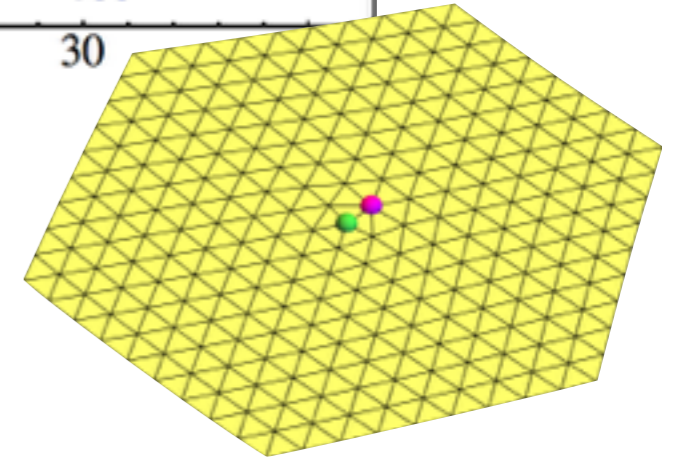
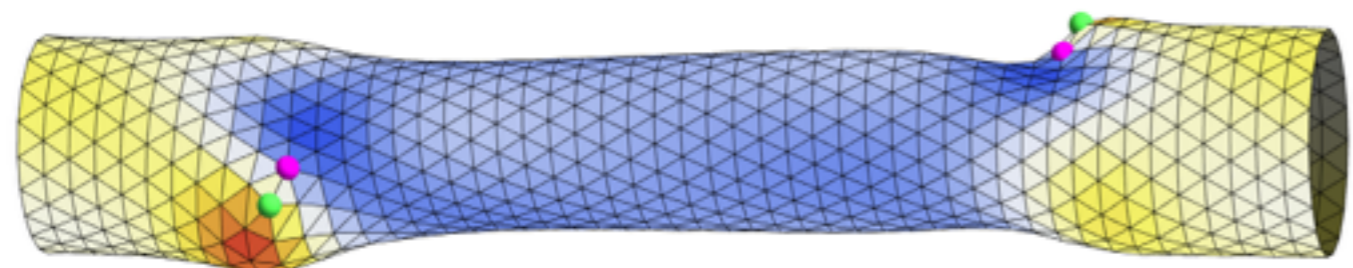
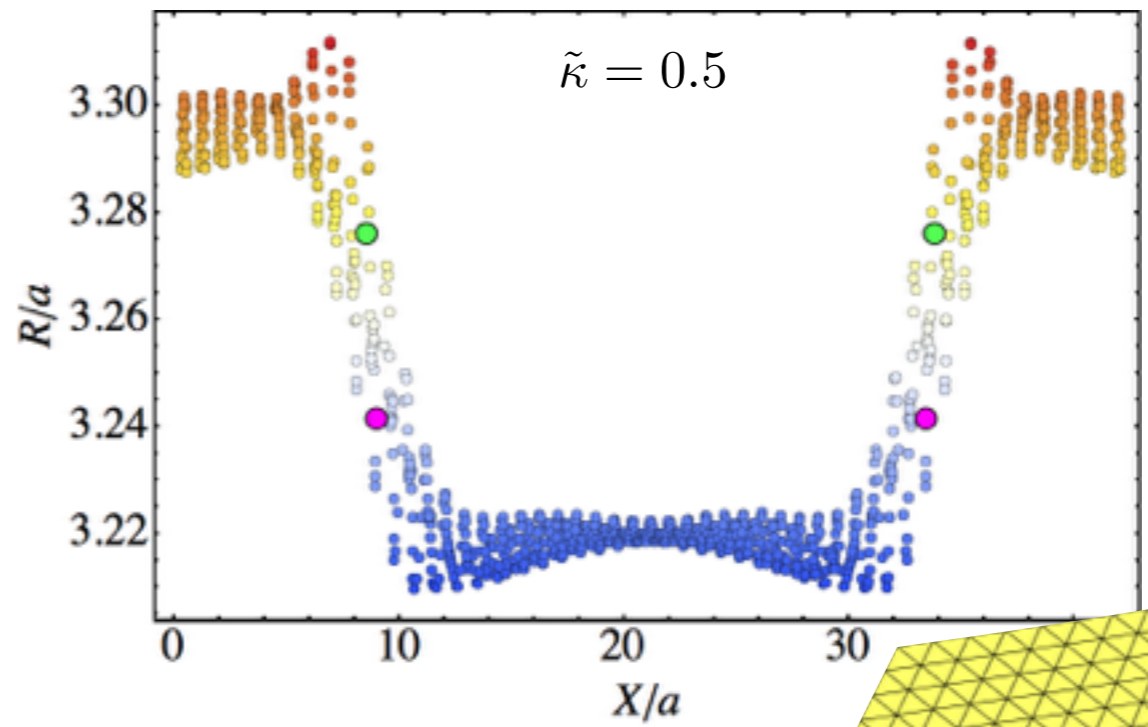
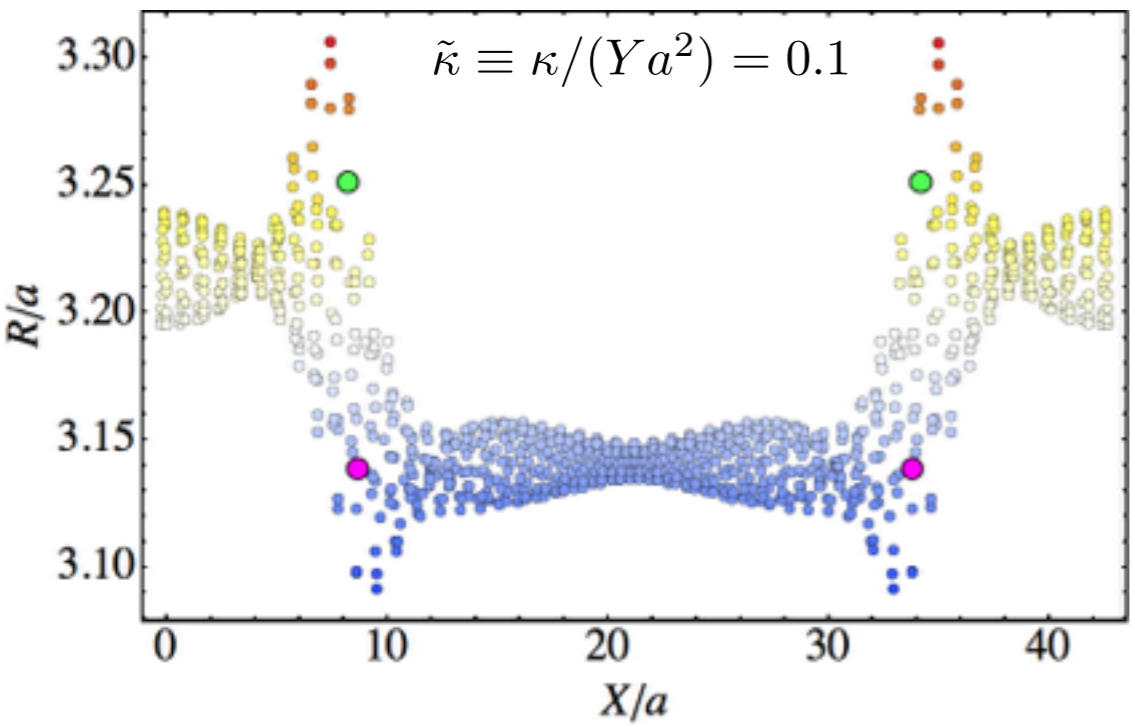
- Large local variations in R can be understood as membrane buckling.
- A membrane with an elementary dislocation at its center buckles when the system size exceeds $\approx (127\tilde{\kappa})a$.
[Seung and Nelson, Phys. Rev. A 38:1005 (1988)]
- For tubes, this predicts buckling when

$$\tilde{\kappa} < \tilde{\kappa}_{\text{buckle}} \equiv 2\pi R_0/127 \quad \rightarrow \approx 0.16 \text{ for } (m, n) = (20, 20)$$



$$\frac{R}{a\tilde{\kappa}} \approx 360$$

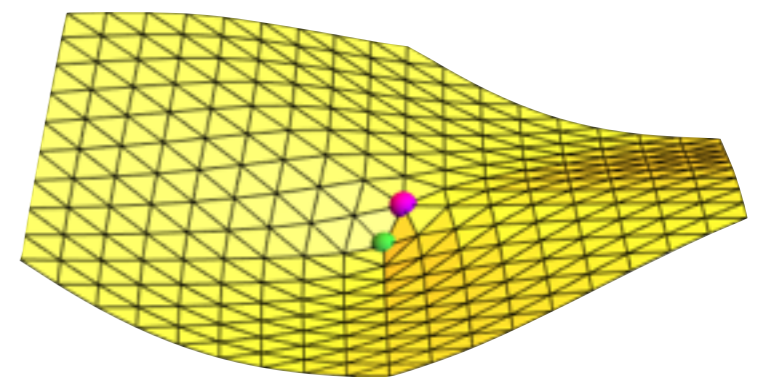
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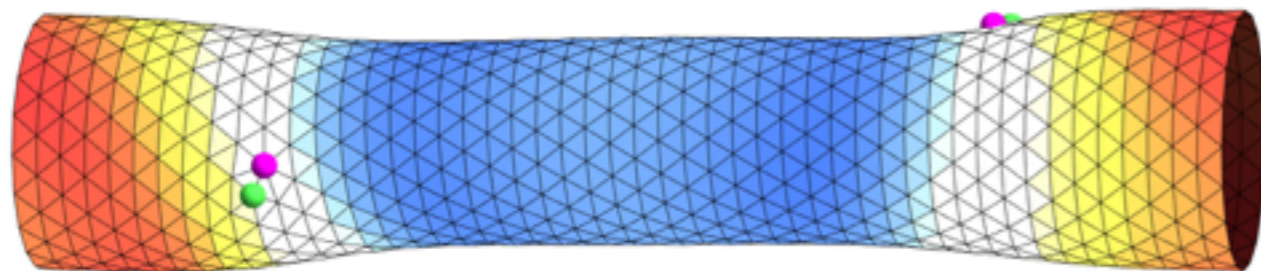
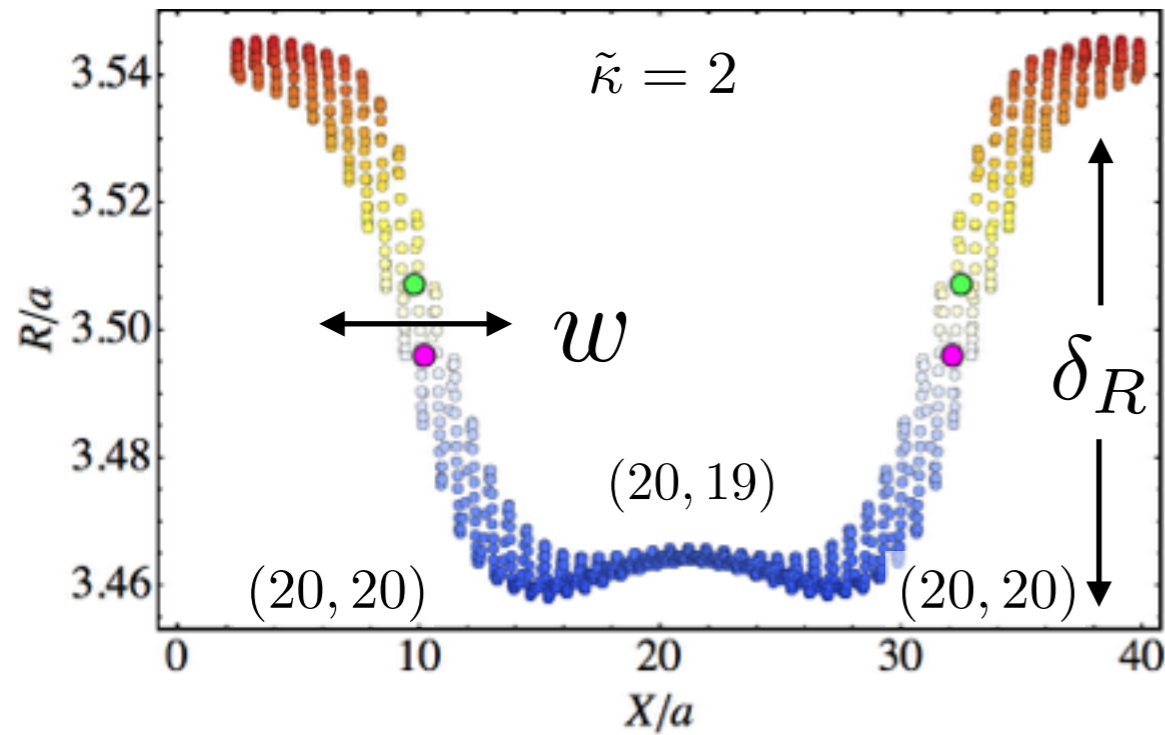


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When there is a well-defined neck profile ($\tilde{\kappa} \gg \tilde{\kappa}_{\text{buckle}}$)...

What is the width of the neck?

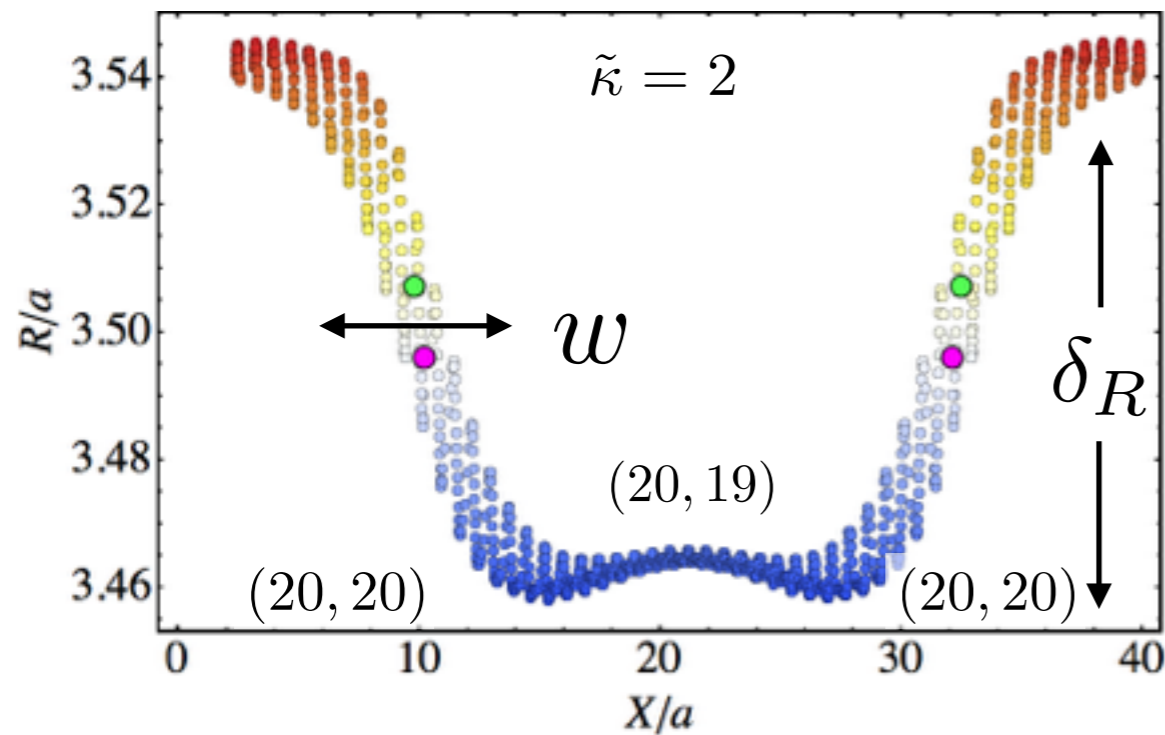


Scaling argument

- $\delta_R \sim a$
- \Rightarrow Stretching energy density $\sim Y(a/R_0)^2$
- Curvature due to neck: a/w^2
- \Rightarrow Bending energy density $\sim \kappa(a/w^2)^2$
- $E_s \sim E_b \Rightarrow w \sim (\kappa/YR_0^2)^{1/4} R_0 = \boxed{\gamma^{-1/4} R_0}$

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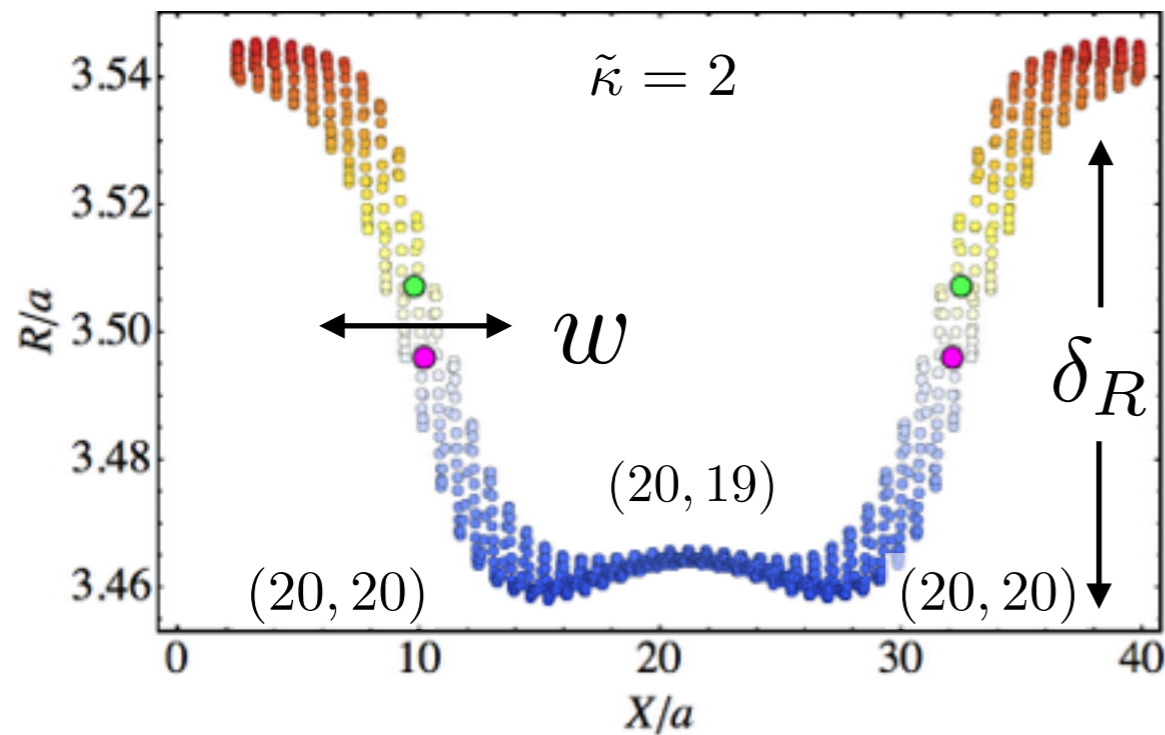
Calculation for a weakly deflected cylinder

- Suppose $R(x) = R_0 + \zeta(x)$, $\zeta \ll R_0$.
- Then $H \approx \partial_x^2 \zeta - R_0^{-1} + R_0^{-2} \zeta$.



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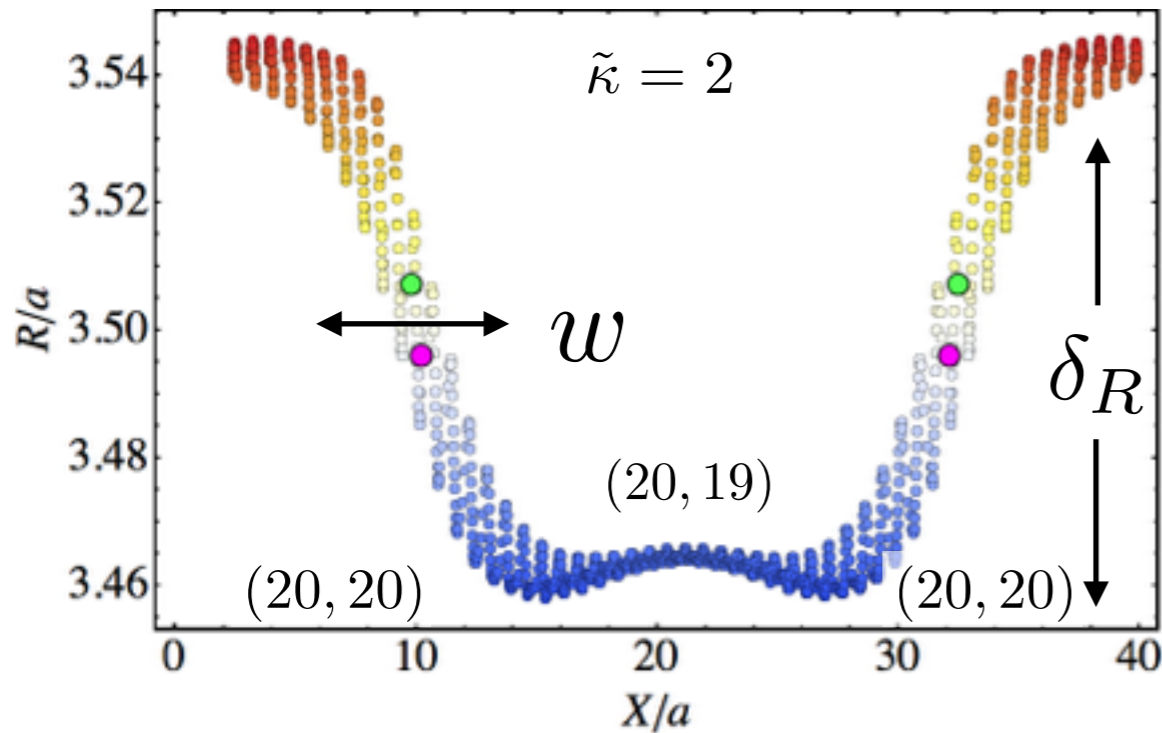


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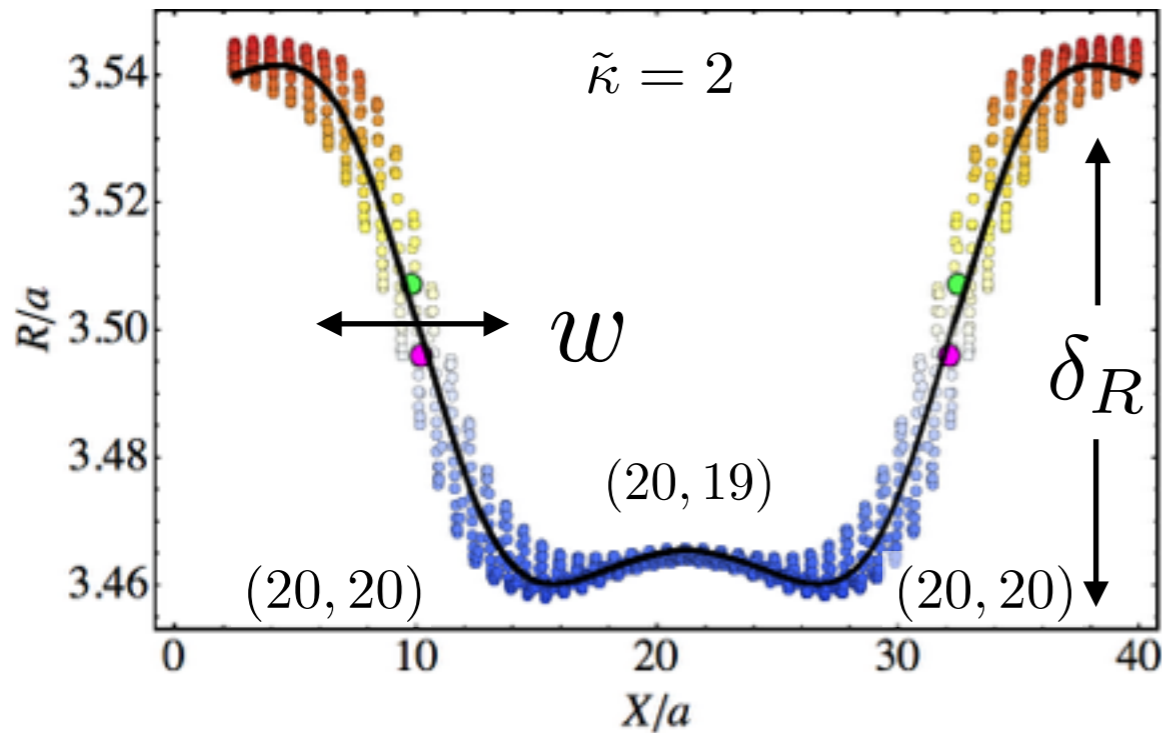
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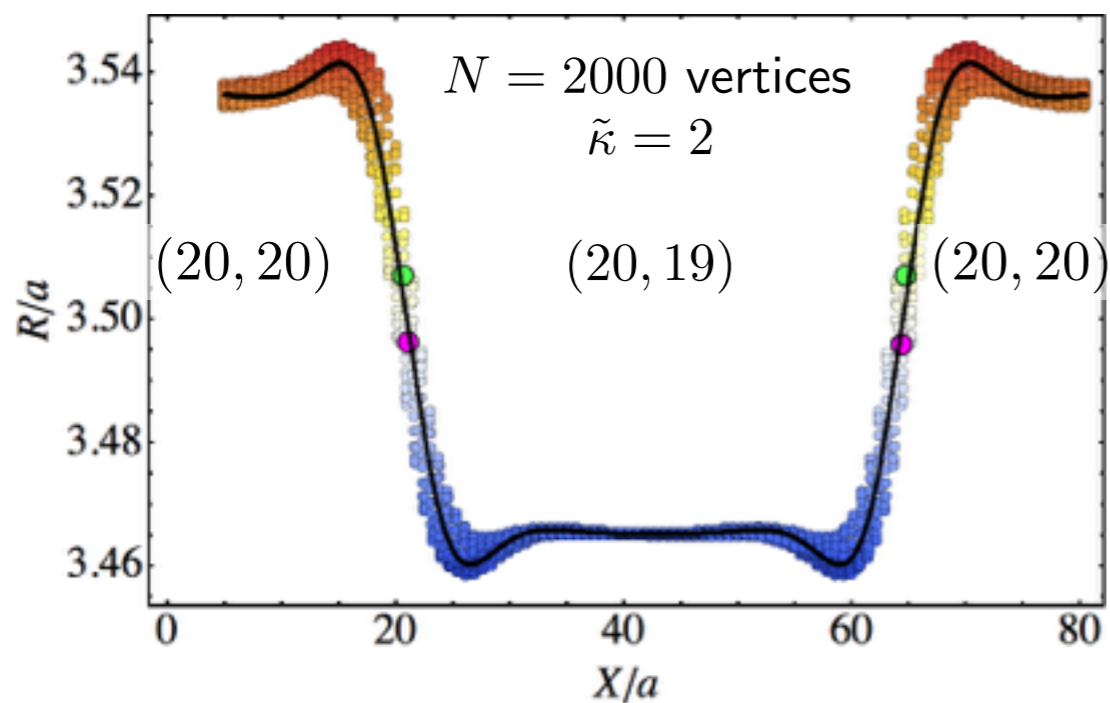
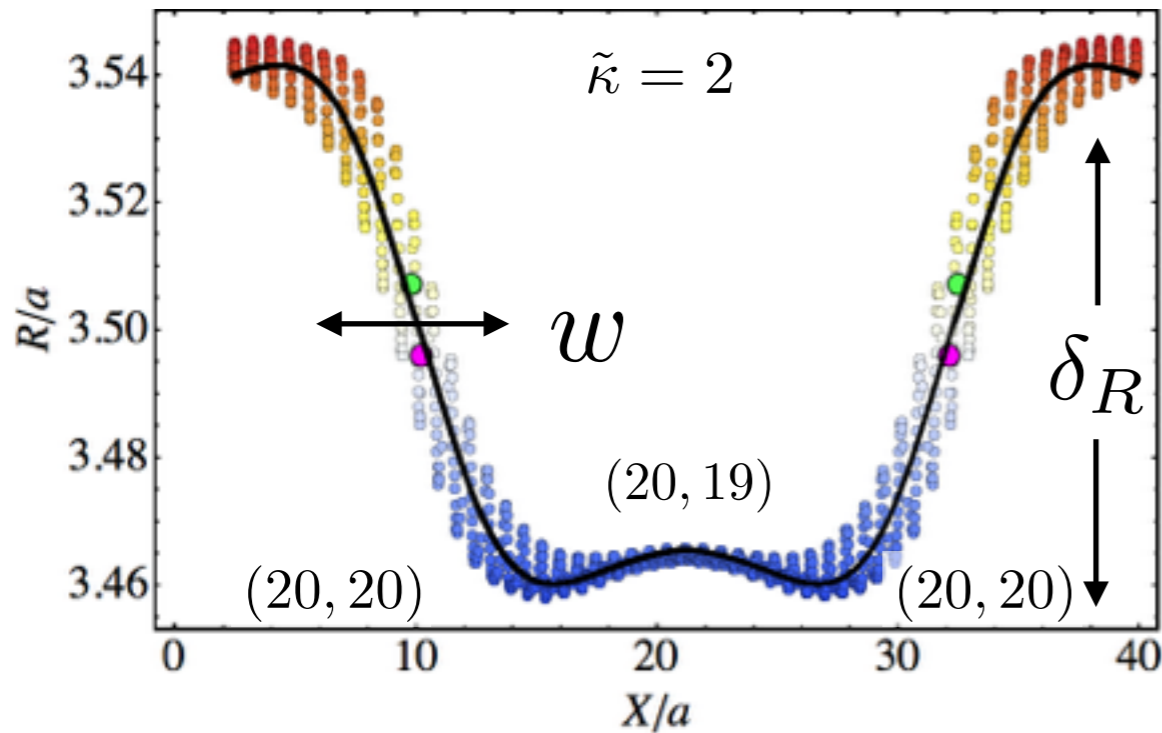
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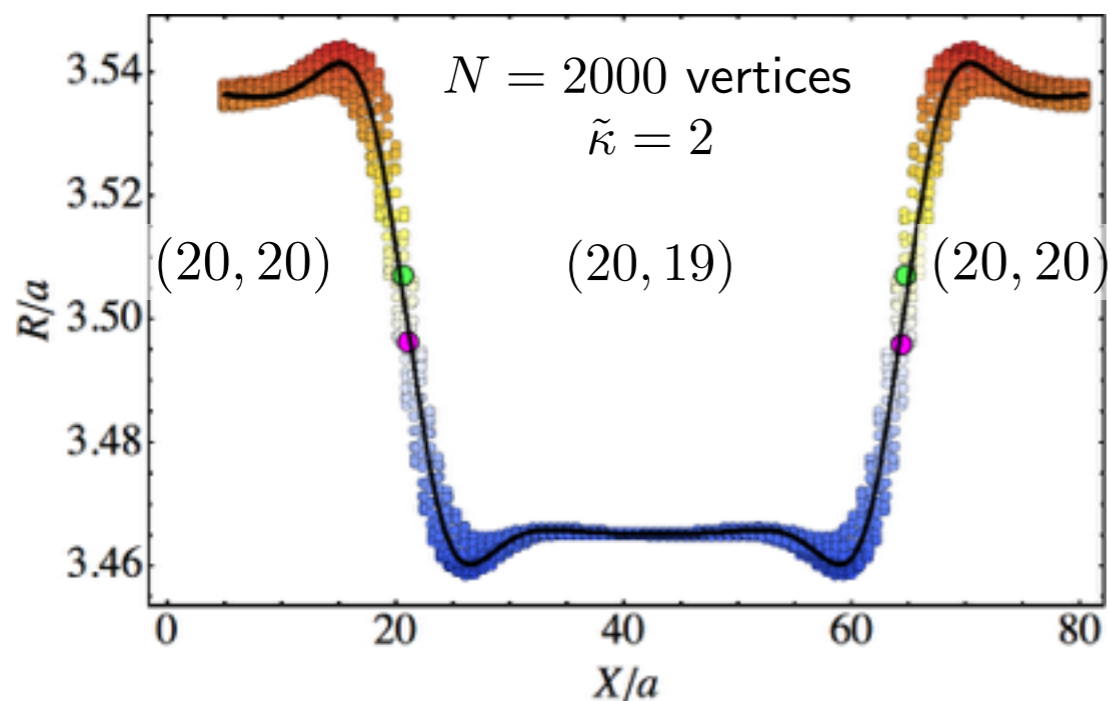
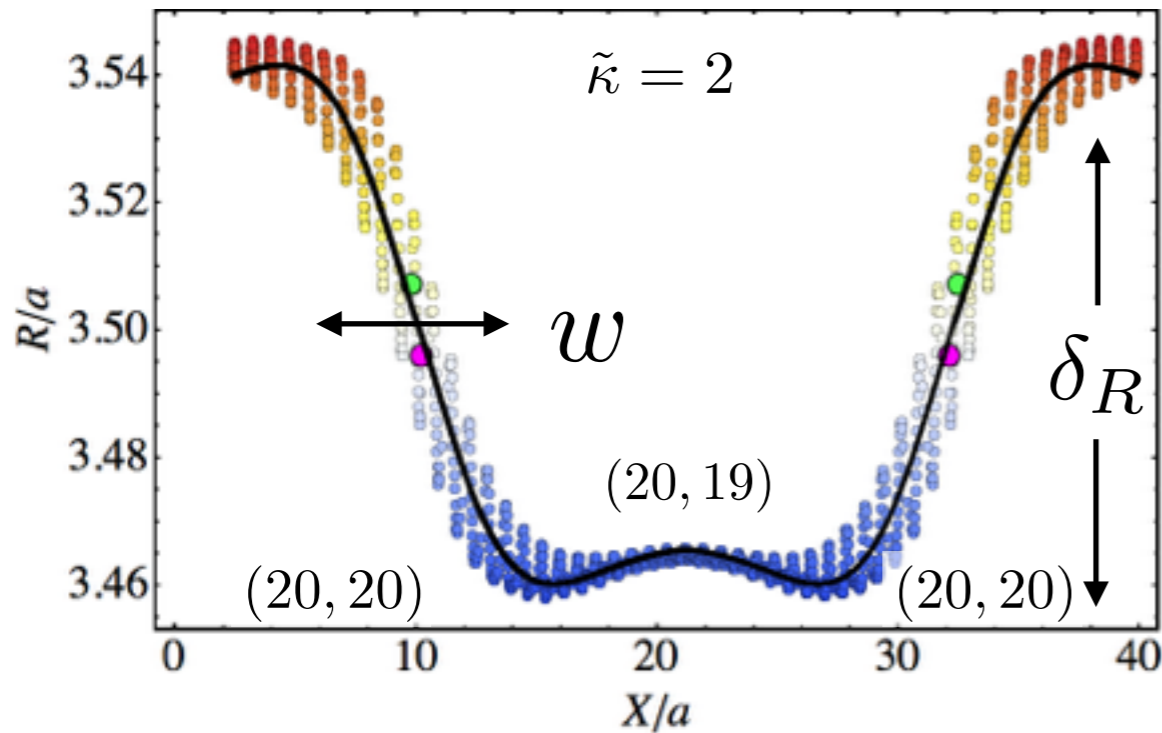
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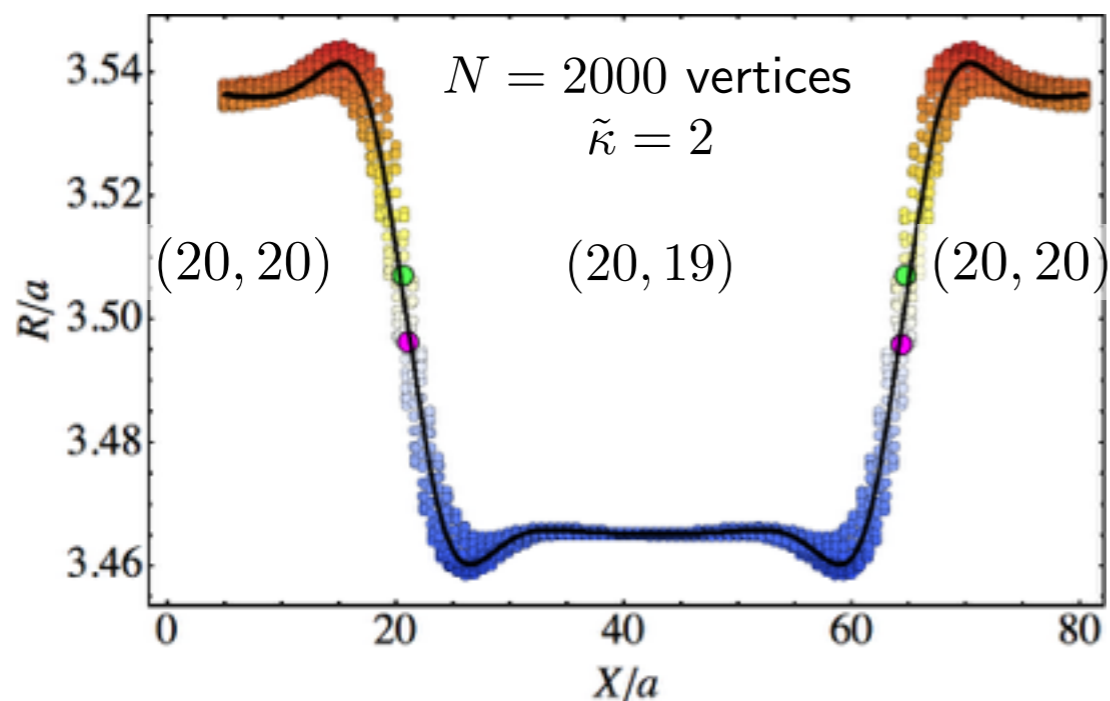
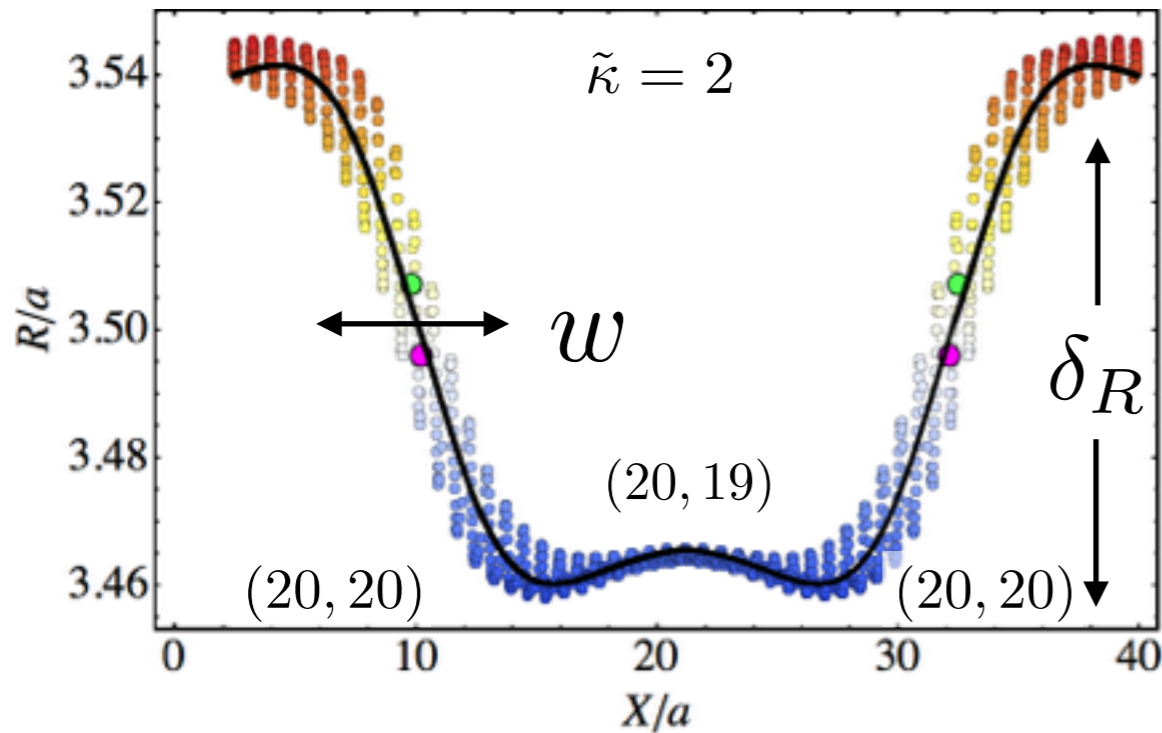
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Conclusions

- Glide separation of dislocation pairs provides a mode of plastic deformation by parastichy transition $(\Delta m, \Delta n)$.
- Tubes under axial tension σ_{xx} converge toward the stable $m = n$ achiral states while their radius shrinks.
- The bending modulus κ shifts up the critical stress σ_{xx}^\dagger required to drive apart dislocations, stabilizing narrow tubes.
 - This shift contains all the R -dependence in σ_{xx}^\dagger .
- If κ is large enough, very small tubes may even be unstable to emission of dislocation pairs that widen the tube.
- The “neck” around a dislocation has width $w \sim \gamma^{-1/4} R$ and also oscillations in local radius.

Acknowledgements

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