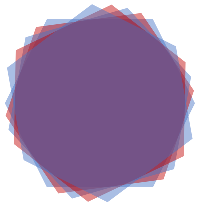
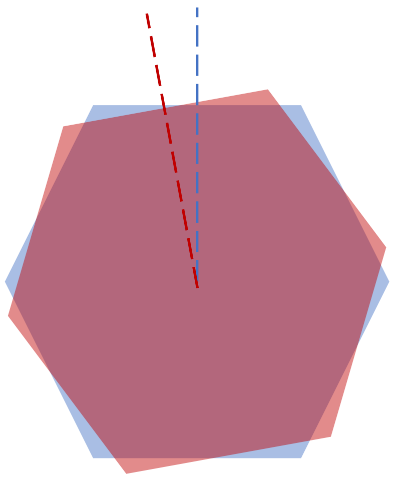
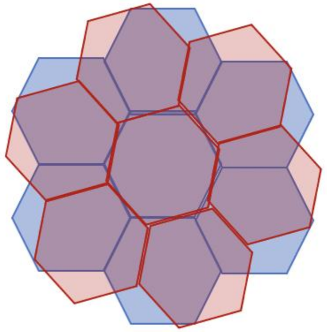
Twist mechanisms of screw dislocation

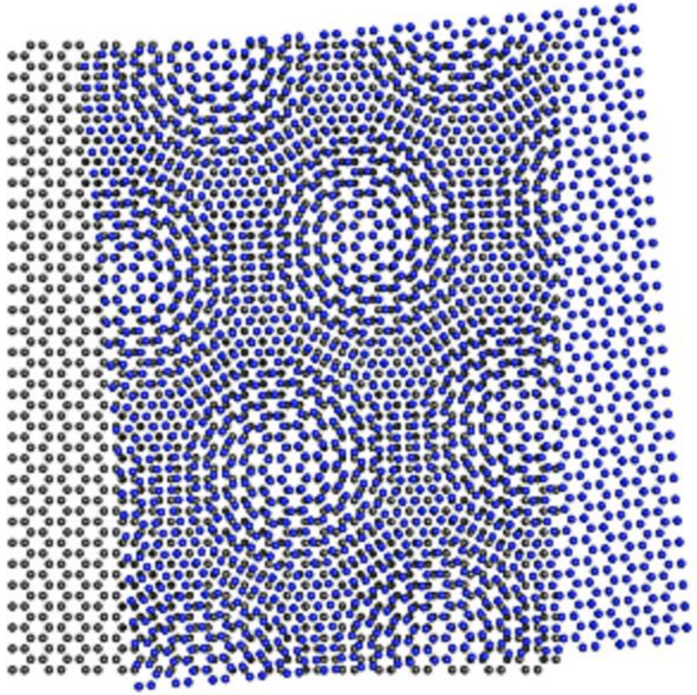


Xin Li 2021-04-11

Twist







artificially manipulate：
growth, peel, transfer, overlaid & rotate

or

screw dislocation growth driven

Moiré patterns appear when two or more periodic grids are overlaid slightly askew,

https://www.nist.gov/news-events/news/2010/04/seeing-moire-graphene

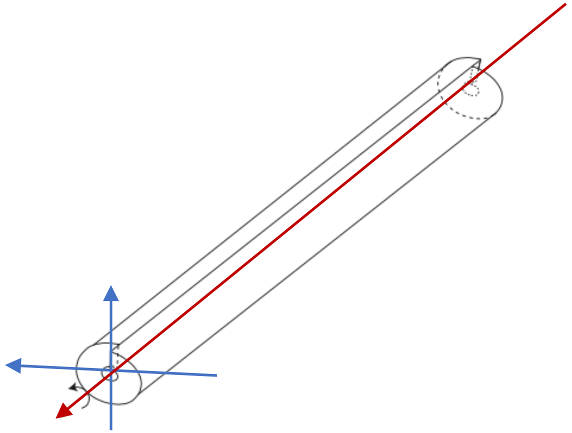
1. Eshelby twist basing on elastic theory

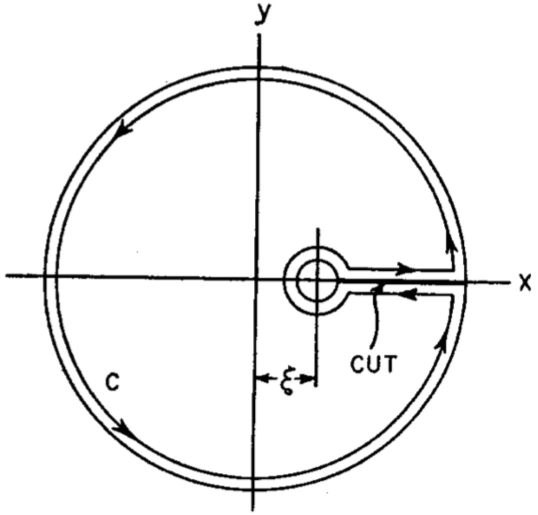
2. non-Euclidean twist basing on non-Euclidean geometry

Eshelby twist

w: *displacement along z direction*

screw dislocation in thin rod





$$w = \frac{b}{2\pi} tan^{-1}\frac{y}{x-\xi} - \frac{b}{2\pi} tan^{-1}\frac{y}{x - R^2/\xi}$$

τ: *stress* $\quad \tau = \mu \nabla w$

M: *torque on cross section*

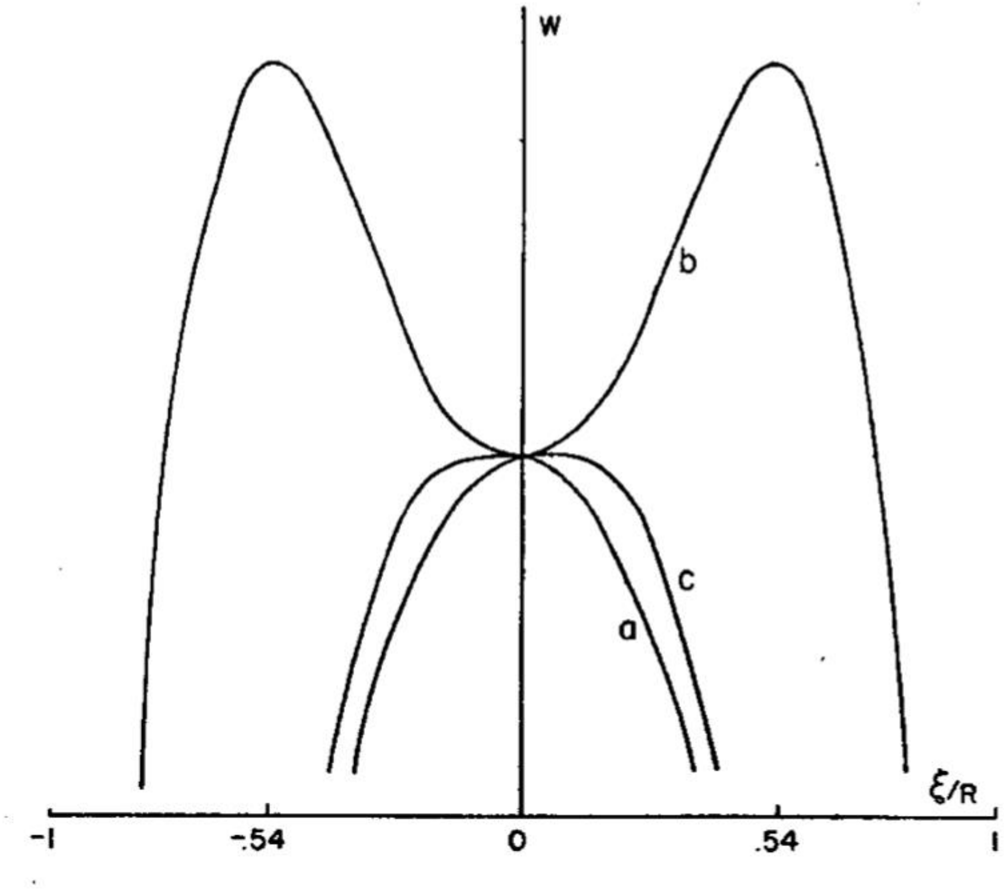
$$M = \mu \int \left(x\frac{\partial w}{\partial y} - y\frac{\partial w}{\partial x}\right) dxdy = \frac{1}{2}\mu b(R^2 - \xi^2)$$

under the limit r_0 *(size of core)* ~ 0

elastic energy: $W = \frac{1}{2}\mu \int (grad\ w)^2 dxdy = \frac{1}{2}\mu \int w\frac{\partial w}{\partial n} ds = \frac{\mu b^2}{4\pi} In(R^2 - \xi^2)$

Image force: $F = -\frac{\partial W}{\partial \xi} = \frac{\mu b^2}{2\pi}\frac{\xi}{R^2-\xi^2}$

Eshelby, J. D. Screw dislocations in thin rods. J. Appl. Phys. 24, 176–179 (1953)



energy of screw dislocation in a cylinder

$$M = \mu \int \left(x\frac{\partial w}{\partial y} - y\frac{\partial w}{\partial x} \right) dxdy = \frac{1}{2}\mu b(R^2 - \xi^2)$$

Twist in cross section of cylinder

J : *torsional constant* $\quad J = \iint x^2\, dA$

$$\theta = \frac{Ml}{\mu J}$$

twist per unit length:

$$\alpha = \frac{\theta}{l} = \frac{M}{\mu\frac{\pi R^4}{2}} = \frac{b}{\pi R^2}\left(1 - \frac{\xi^2}{R^2}\right) \sim \frac{1}{R^2}$$

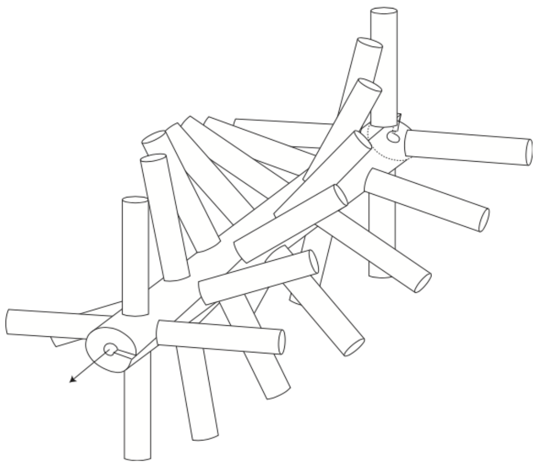
obvious in nano wir

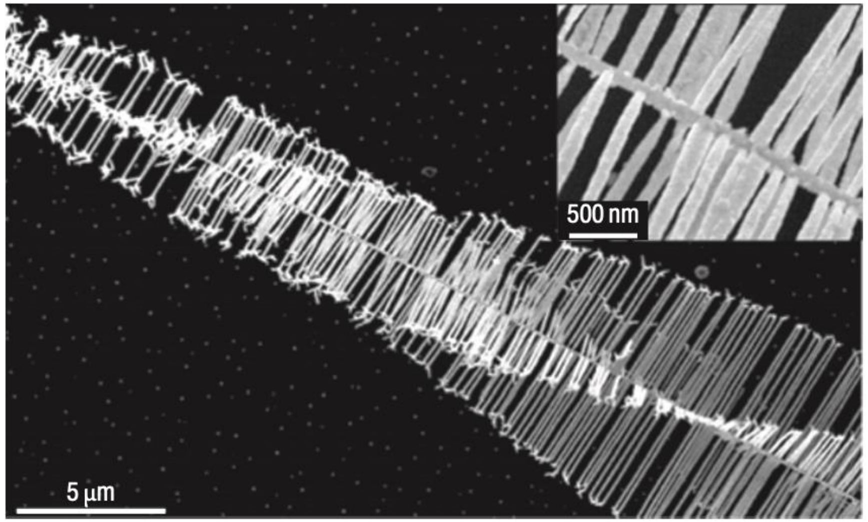
$$W = \frac{\mu b^2}{4\pi}\left[In(R^2 - \xi^2) - \frac{(R^2 - \xi^2)^2}{R^4} \right]$$

$$\frac{1}{2}\alpha M$$

Eshelby, J. D. Screw dislocations in thin rods. J. Appl. Phys. 24, 176–179 (1953)

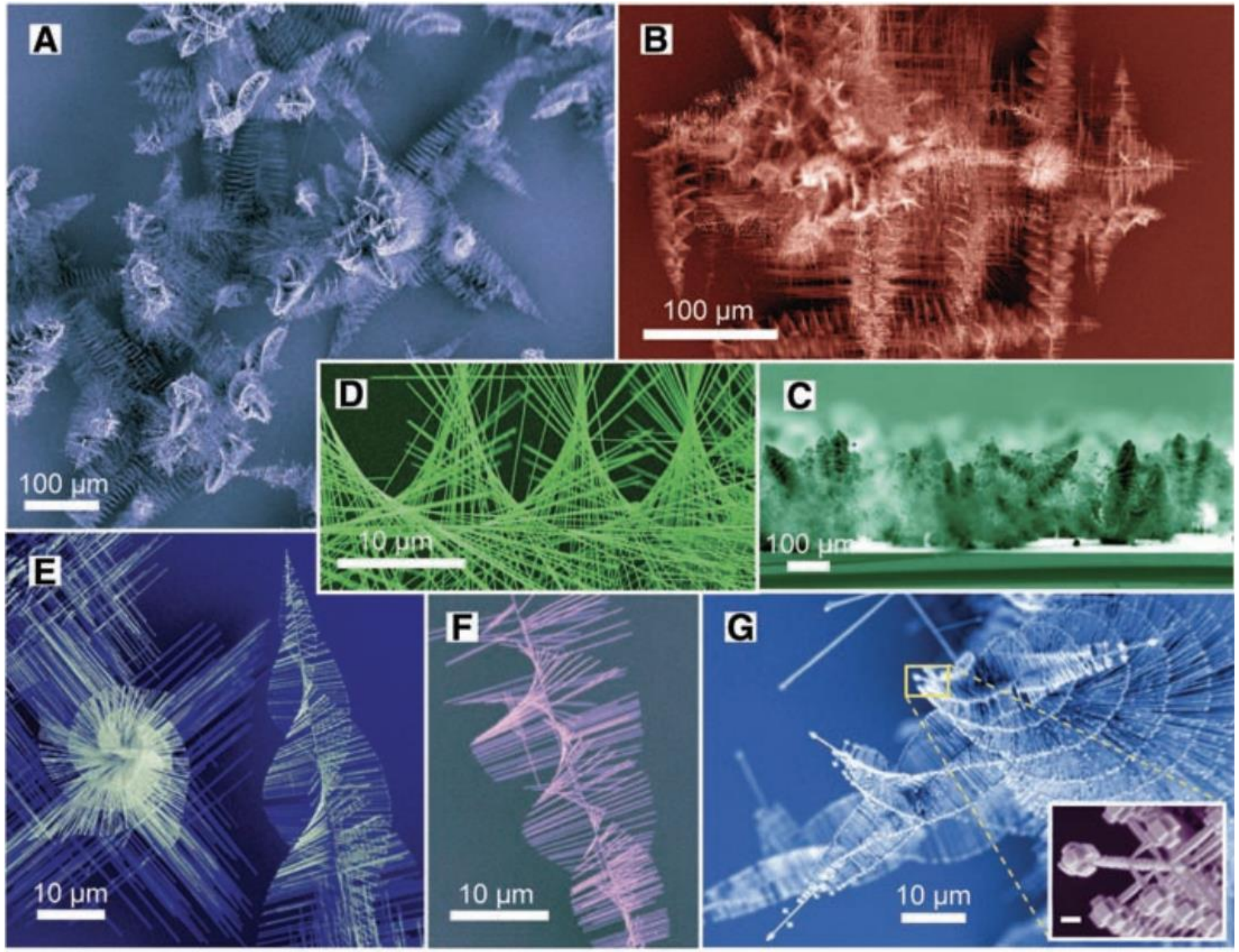
Eshelby twist in nanowire





singe chiral branch of PbSe nanowire

Zhu, J., Yi,C. *et al. Nature Nanotech* **3,** 477–481 (2008).



SEM micrpgraphs of PbS pin tree nanowires

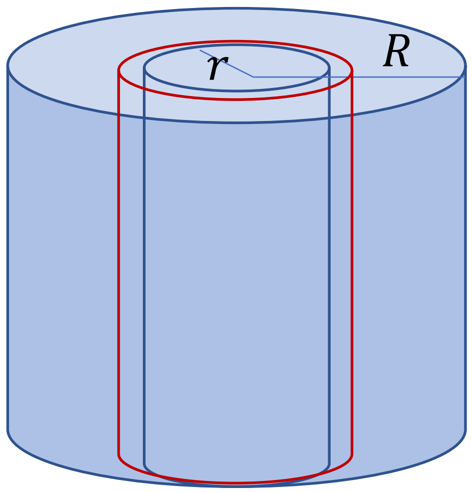
Bierman, M. J.; Jin, S, Science 2008, 320, 1060-1063

Eshelby twist (consider **inner surface energy**)

strain energy density

dislocation strain energy $E = \frac{\mu b^2}{4\pi} \ln\left(\frac{R}{r}\right) = \int_r^R 2\pi r * u dr$

$$u = \frac{\mu b^2}{8\pi^2} \frac{1}{r^2}$$

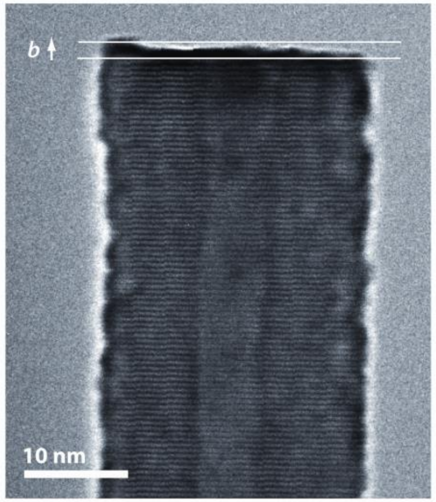


suppose inner surface evaporate thickness dr

$$dW = 2\pi\gamma dr - \frac{\mu b^2}{8\pi^2} \frac{1}{r^2} * 2\pi r dr$$

$$\frac{dW}{dr} = 0 \longrightarrow 2\pi\gamma = \frac{\mu b^2}{4\pi} \frac{1}{r}$$

$$b_{tube} = \sqrt{\frac{8\pi^2 \gamma r}{\mu}}$$



ZnO nanotube

$$\alpha = \frac{\theta}{l} = \frac{b}{\pi R^2 + \pi r^2}$$

competion mechanism for alleviation of dislocation strain

(i) forming hollow core. (ii) Eshelby twist

$$\mathrm{E} = 2\pi\gamma r + \frac{\mu b^2}{4\pi} \ln\left(\frac{R}{r}\right) - \frac{\mu b^2}{4\pi} \frac{R^2 - r^2}{R^2 + r^2}$$

F. C. Frank, Acta Crystallogr. 4, 497 (1951)

Stephen A. Morin, Song Jin. Science 2010,328, 5977

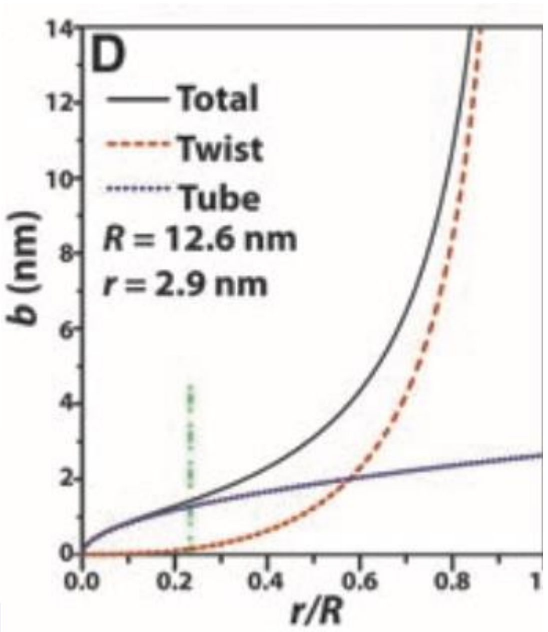
$$E = 2\pi\gamma r + \frac{\mu b^2}{4\pi}\ln\left(\frac{R}{r}\right) - \frac{\mu b^2}{4\pi}\frac{R^2 - r^2}{R^2 + r^2}$$

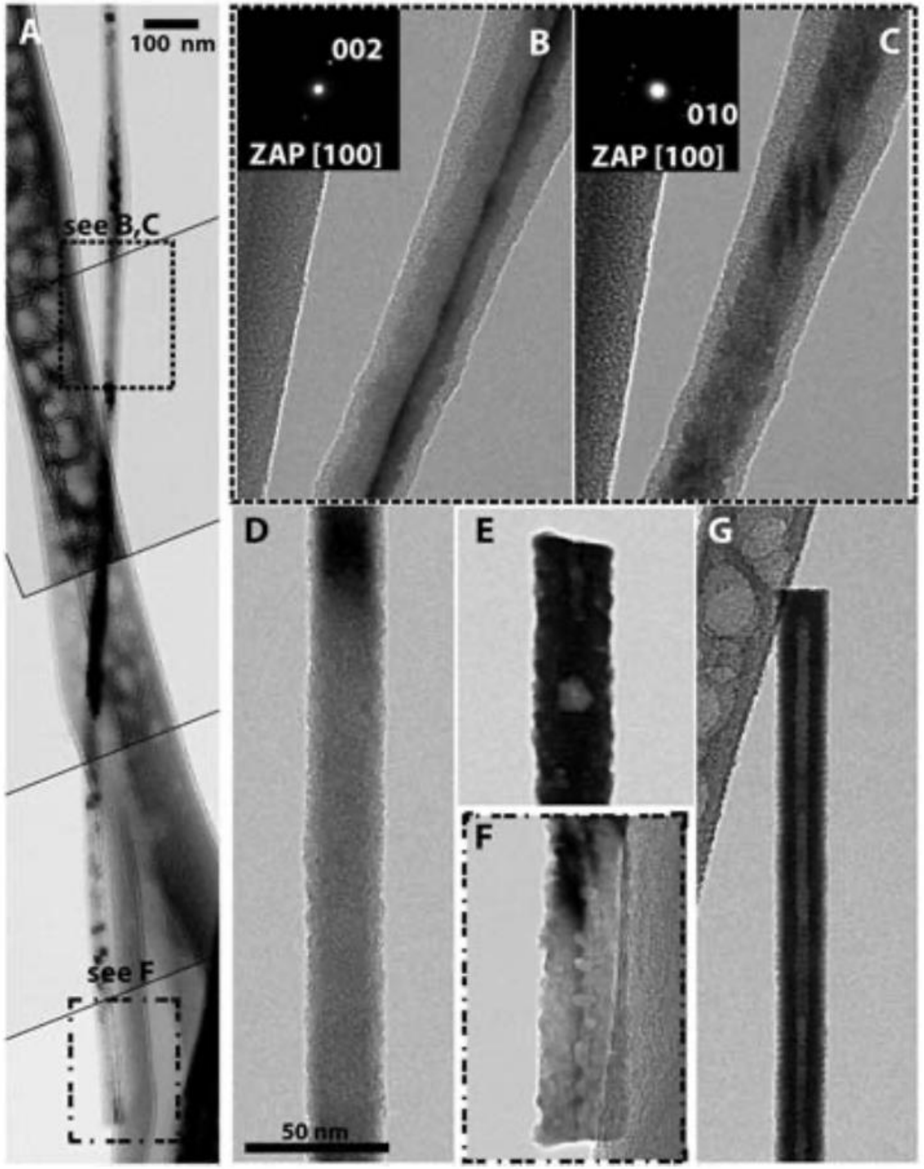
$$\frac{dE}{dr} = 0$$

$$b_{total} = \sqrt{\frac{8\pi^2\gamma r}{\mu}\left(\frac{R^2 - r^2}{R^2 + r^2}\right)}$$

$$\boldsymbol{b_{twist}} = b_{total} - \mathrm{b_{tube}} = \sqrt{\frac{8\pi^2\gamma r}{\mu}\left(\frac{R^2 + r^2}{R^2 - r^2} - 1\right)}$$

$$b_{tube} = \sqrt{\frac{8\pi^2\gamma r}{\mu}}$$

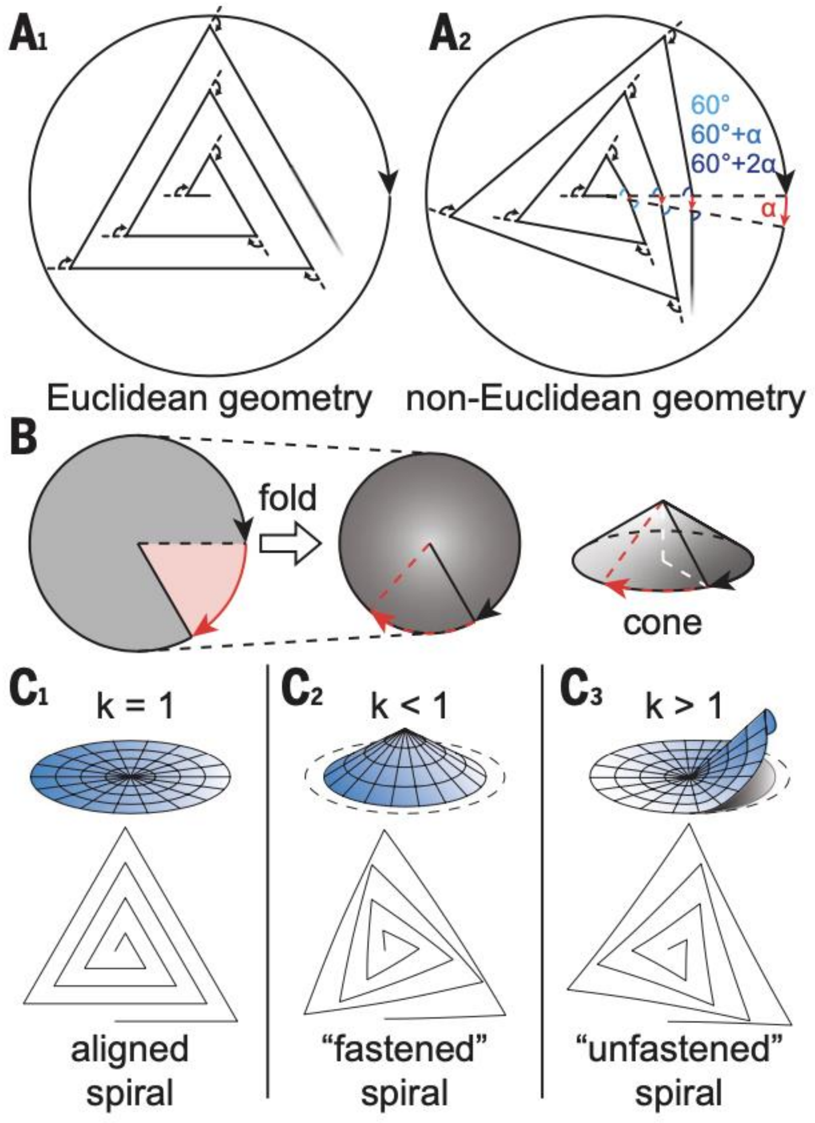




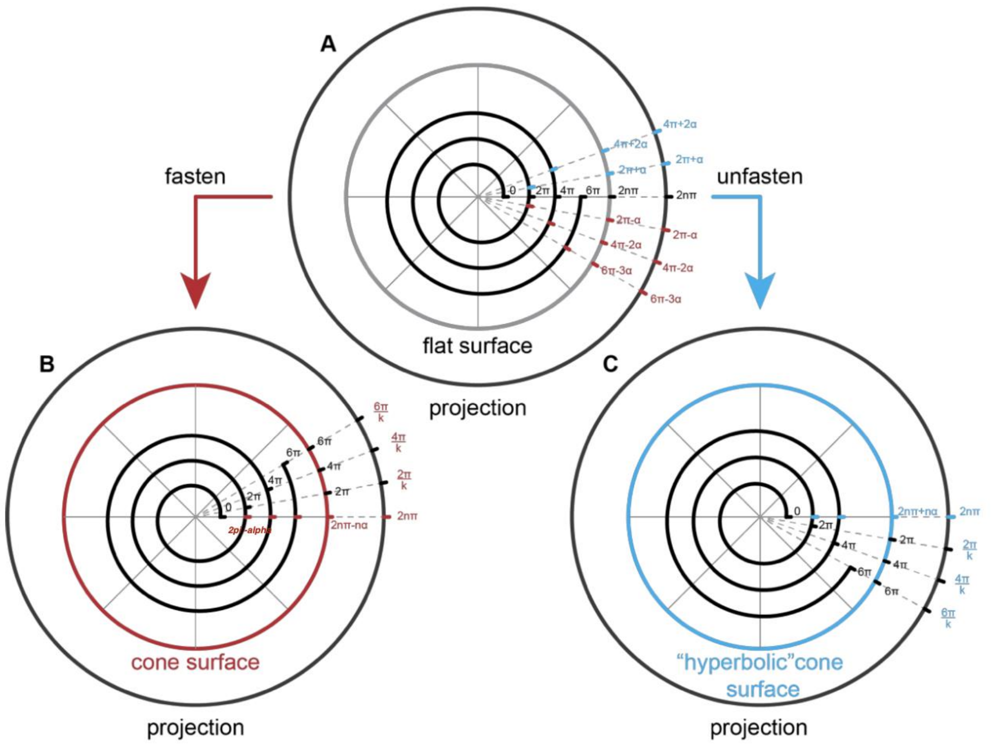
TEM observation of screw dis- locations within ZnO NWs and the crystal behavior of NTs.

Stephen A. Morin, Song Jin. Science 2010,328, 5977

non-Euclidean twist



Triangular dislocation spiral on Euclidean and non-Euclidean surfaces illustrating the twisting process.



$$r_{proj} = k r_{c.s}$$

$$\theta_{proj} = \frac{\theta_{c.s}}{k}$$

Yuzhou Zhao, Song Jin, Science 2020, 370, 6515, 442-445 euqation of triangle spirals

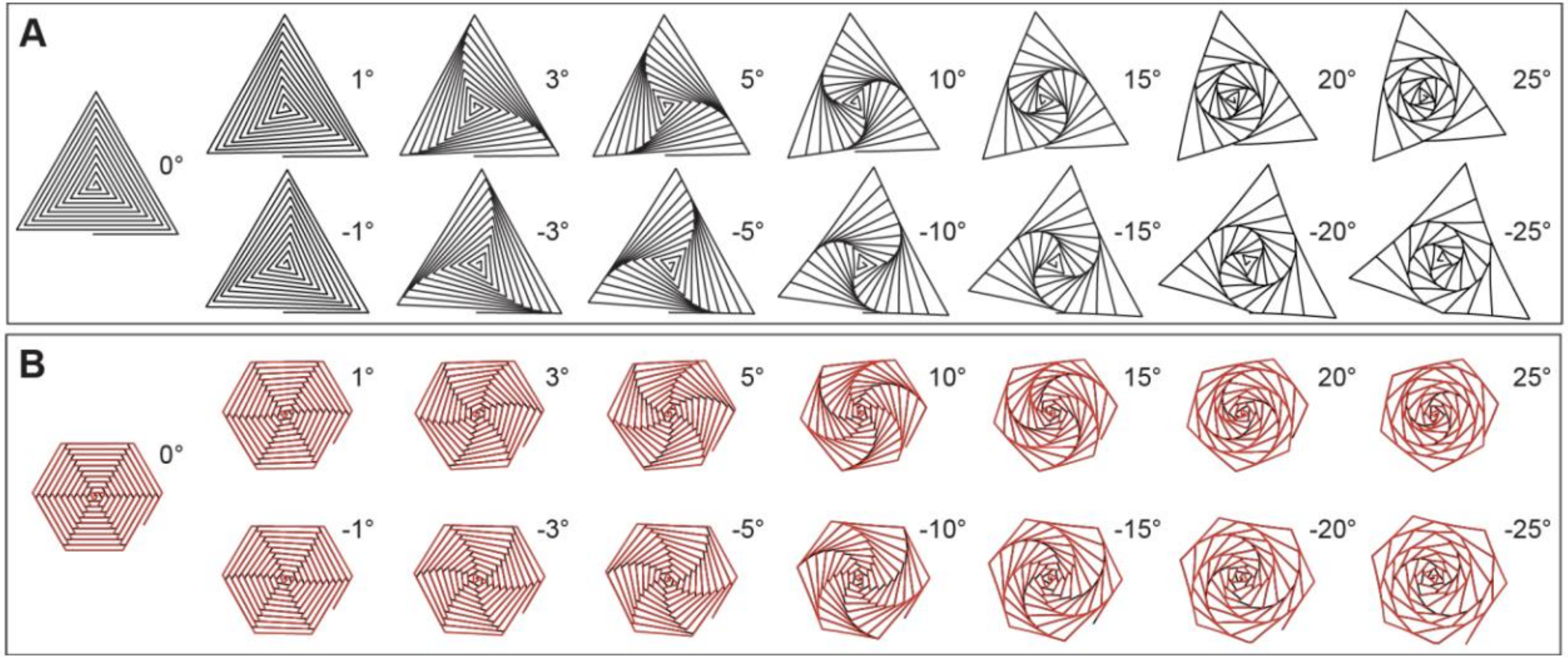
$$r = \begin{cases} \frac{n}{\cos\left(\pm\theta+\frac{2\pi}{3}+2n\pi\right)} & -\pi + 2n\pi \le \pm\theta \le -\frac{\pi}{3} + 2n\pi \\ \frac{n}{\cos(\pm\theta+2n\pi)} & -\frac{\pi}{3} + 2n\pi \le \pm\theta \le \beta \\ \frac{n+1}{\cos\left(\pm\theta-\frac{2\pi}{3}+2n\pi\right)} & \beta \le \pm\theta \le \pi + 2n\pi \end{cases}$$

$$r_{proj} = kr_{c.s}$$

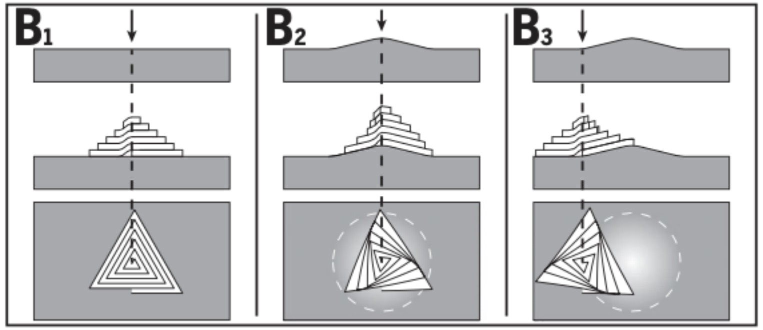
$$\theta_{proj} = \frac{\theta_{c.s}}{k}$$

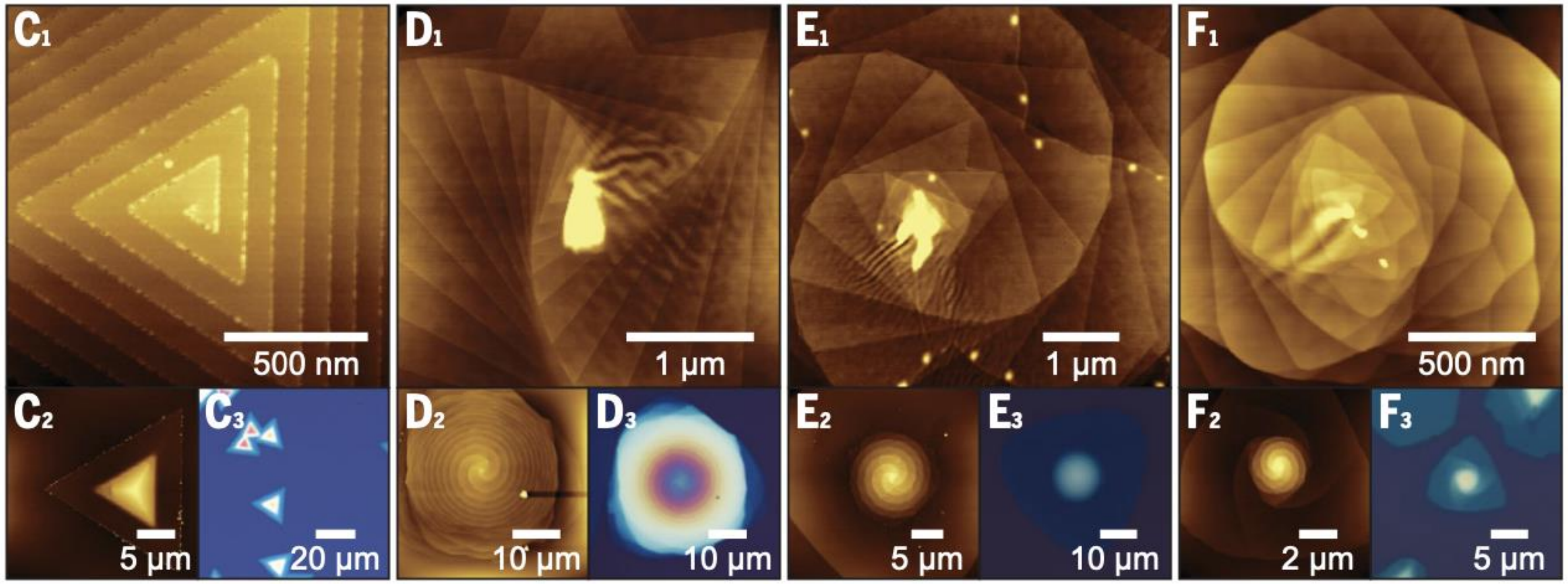
euqation of projection of triangle spirals

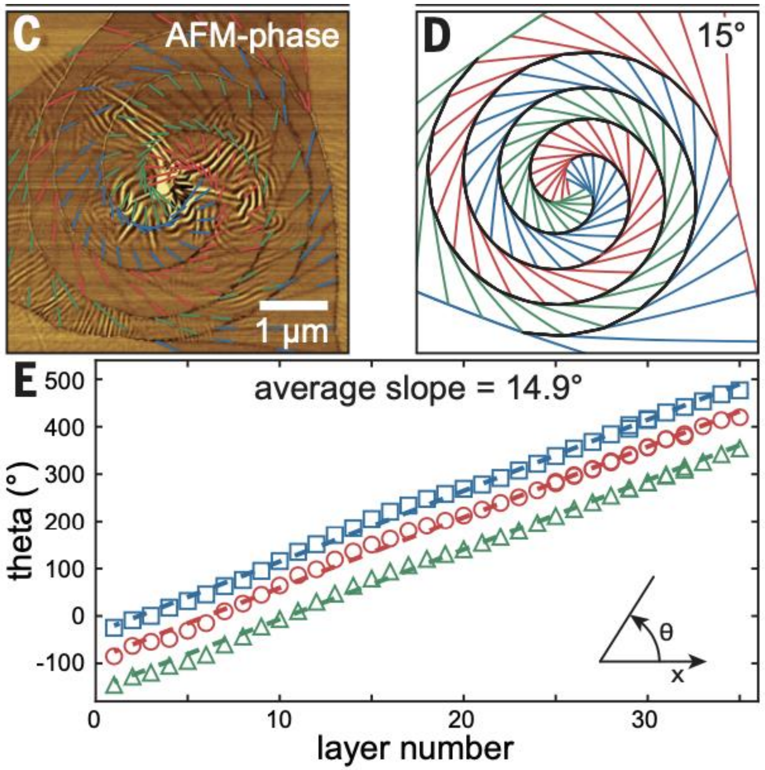
$$r' = \begin{cases} \frac{nk}{\cos\left(\pm k\theta'+\frac{2\pi}{3}+2n\pi\right)} & \frac{1}{k}(-\pi + 2n\pi) \le \pm\theta' \le \frac{1}{k}(-\frac{\pi}{3} + 2n\pi) \\ \frac{nk}{\cos(\pm k\theta'+2n\pi)} & \frac{1}{k}(-\frac{\pi}{3} + 2n\pi) \le \pm\theta' \le \beta' \\ \frac{(n+1)k}{\cos\left(\pm k\theta'-\frac{2\pi}{3}+2n\pi\right)} & \beta' \le \pm\theta' \le \frac{1}{k}(\pi + 2n\pi) \end{cases}$$



Simulated shapes of triangular and hexagonal supertwisted spirals with right-handed screw dislocations and different twist angles.







Experimental demonstration of supertwisted spirals on non-Euclidean surfaces

Yuzhou Zhao, Song Jin, Science 2020, 370, 6515, 442-445 for spirals without triangle shape

single spiral

$$r = \alpha(\theta - \theta_1) + c$$

left hand

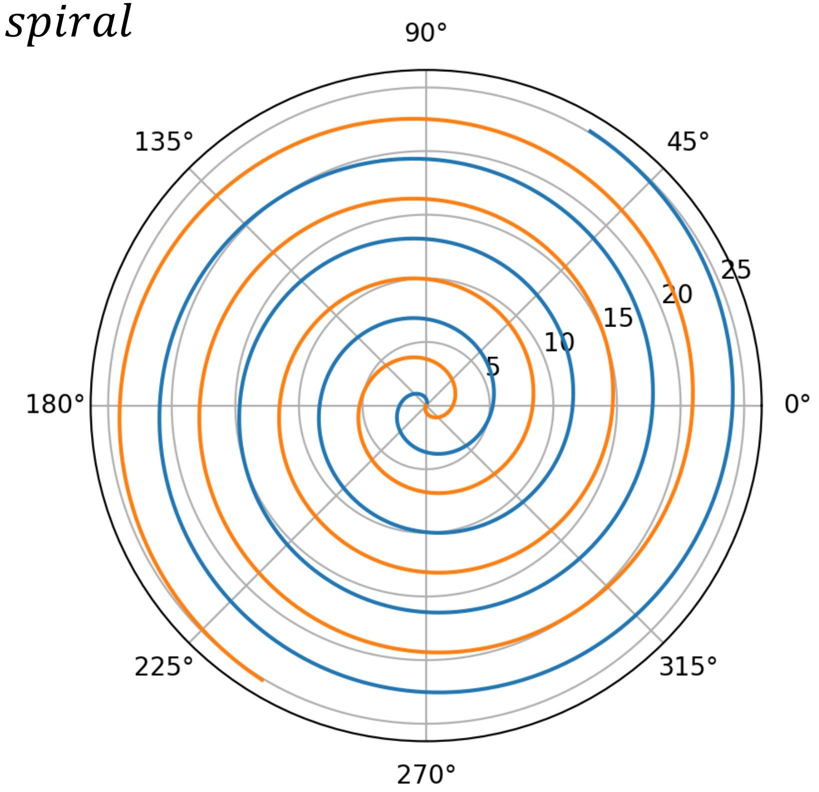
$$\theta_1 + 2(n-1)\pi < \theta < \theta_1 + 2n\pi$$

$$r = \alpha(\theta_1 - \theta) + c$$

right hand

$$\theta_1 - 2n\pi < \theta < \theta_1 - 2(n-1)\pi$$

double spiral



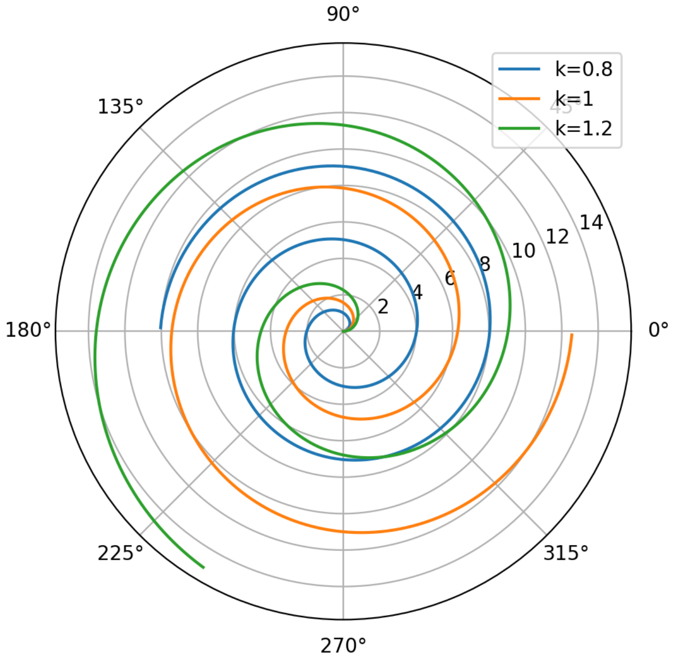
twisted single spiral

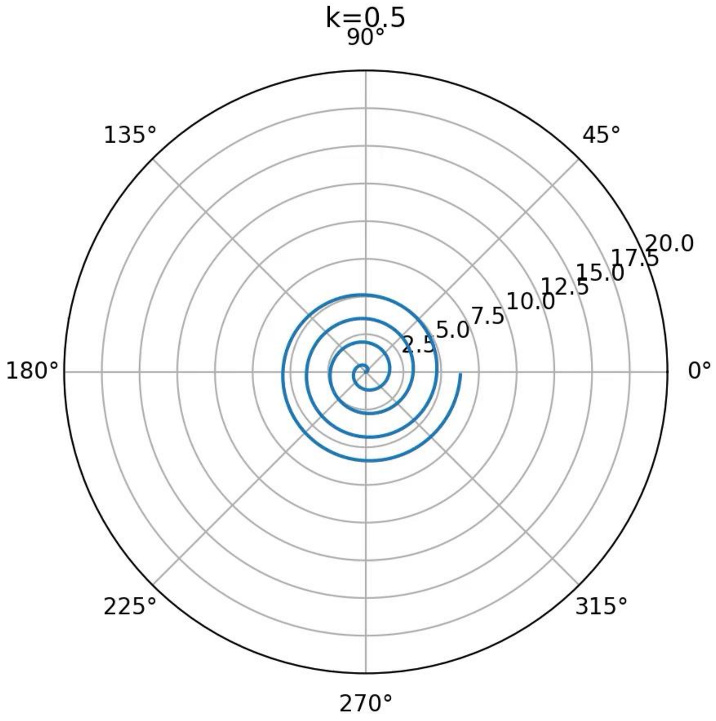
$$r' = k(\alpha(k\theta' - \theta_1) + c) \qquad \frac{\theta_1 + 2(n-1)\pi}{k} < \theta' < \frac{\theta_1 + 2n\pi}{k} \qquad \text{left hand}$$

$$r' = k(\alpha(\theta_1 - k\theta') + c) \qquad \frac{\theta_1 - 2n\pi}{k} < \theta' < \frac{\theta_1 - 2(n-1)\pi}{k} \qquad \text{right hand}$$

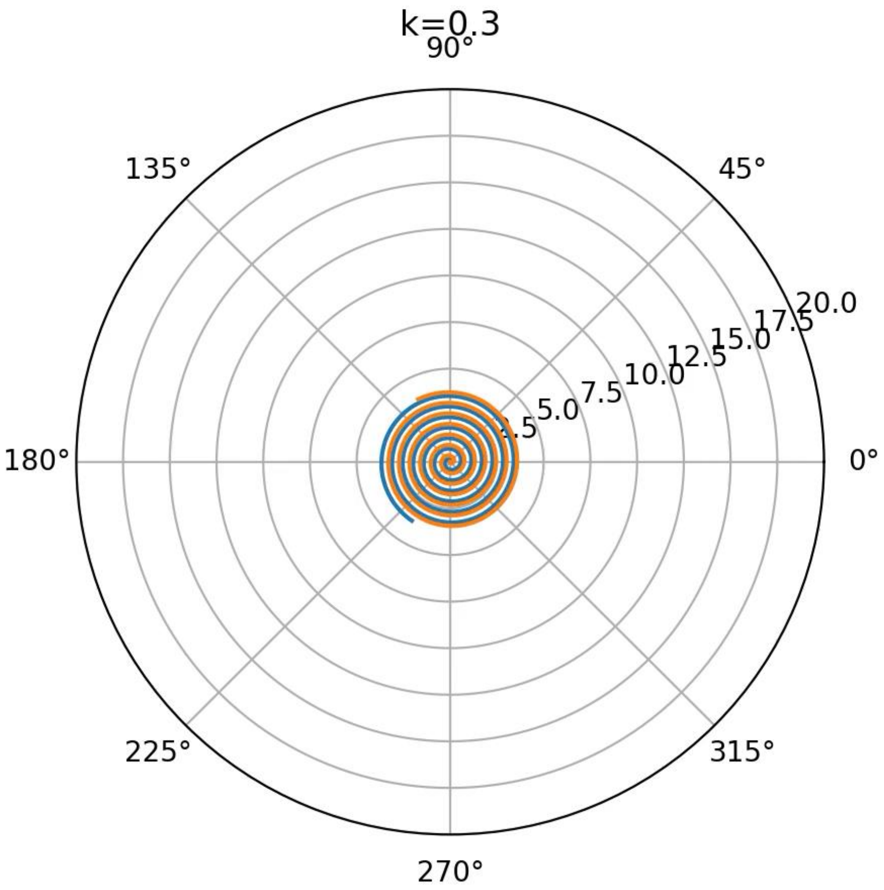
$$r_{proj} = k r_{c.s}$$

$$\theta_{proj} = \frac{\theta_{c.s}}{k}$$





twisted double spiral



Summary:

1. Eshelby twist : free energy reduction from twist, applied to NW,NT

2. non-Euclidean twist : geometrical restriction of curved surface, apply to any 2D material

3. Twist mechanisms reflect discrepancy between continuum elastic theory and crystallography.