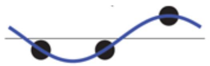
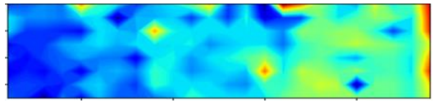
Topological stripe domain in hexagonal ferrites basing on quantitative analysis of atom displacement

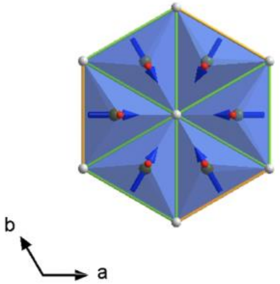


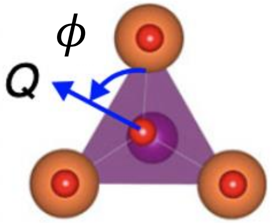


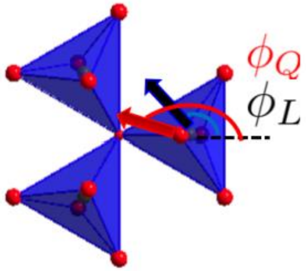
Xin Li 2020.06.12

Structural Distortion （K_3 and Γ_2^-）

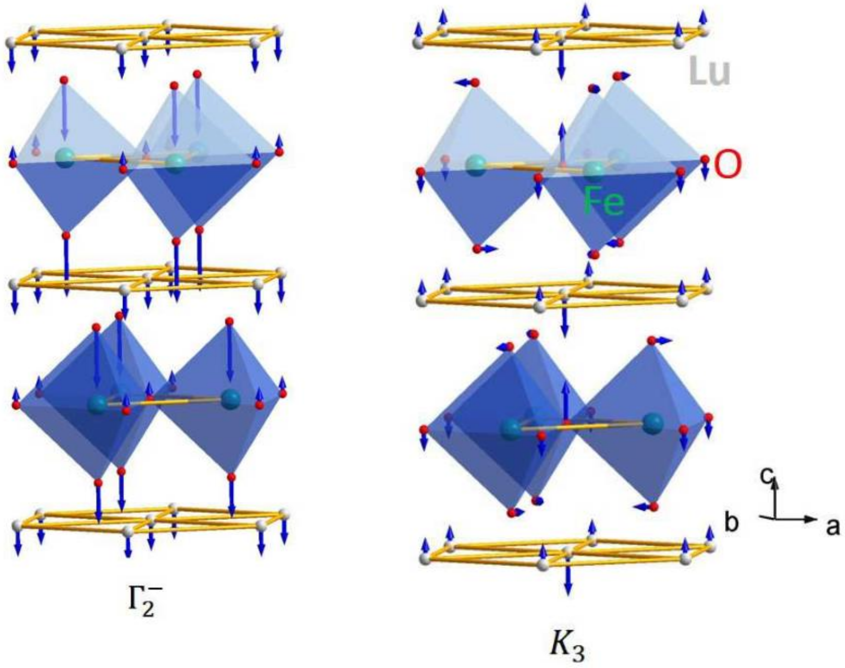
view from [001] direction
displacement of apex oxygen



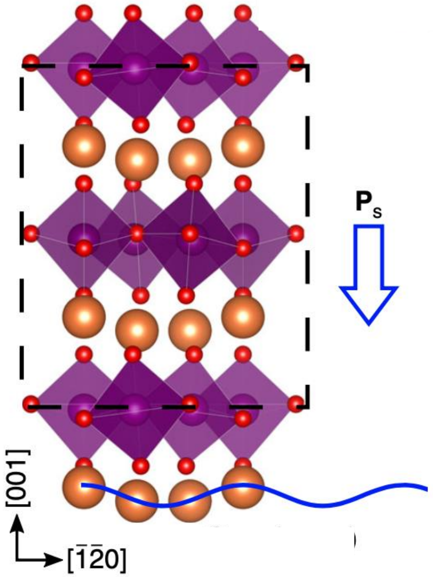


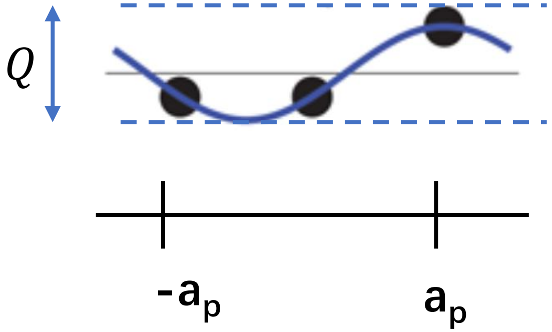


$Q = (Q_1, Q_2) = (Q\cos\phi, Q\sin\phi)$



view from [1-1 0] direction
displacement of rare earth





$$u(\boldsymbol{r_n}) = u_0 + Q_1 \cos \boldsymbol{q} \cdot \boldsymbol{r_n} + Q_2 sin\ \boldsymbol{q} \cdot \boldsymbol{r_n}$$

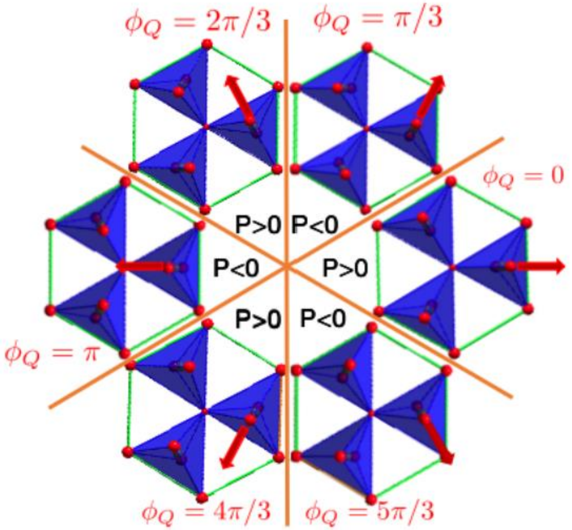
Γ_2^- K_3

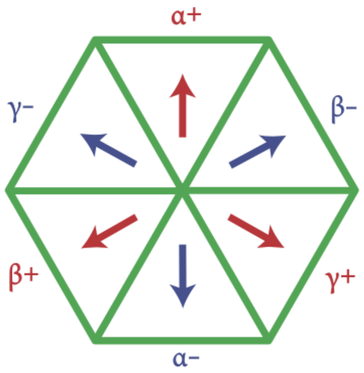
$$u = Qcos(q \cdot r - \phi)$$

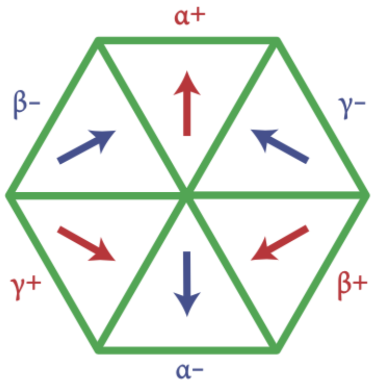
Structural Domain

view from [001] direction

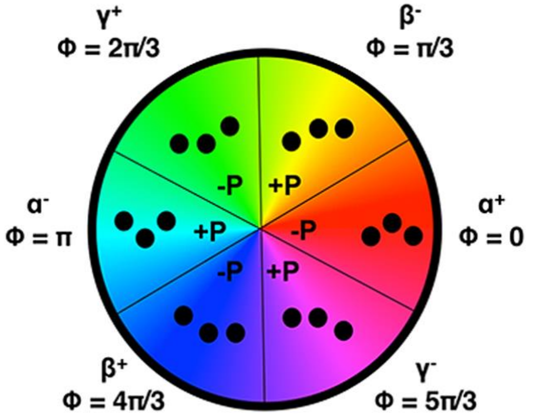
$$\phi=\phi_Q-\frac{\pi}{3}$$

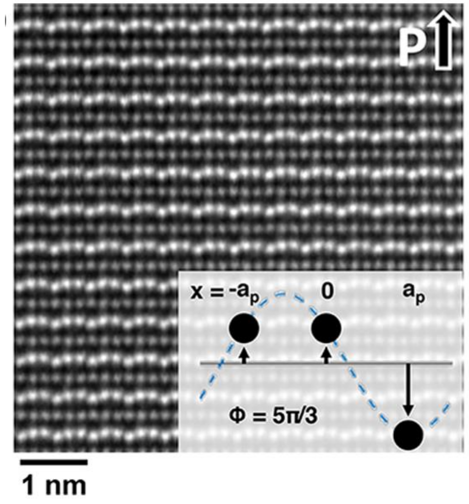


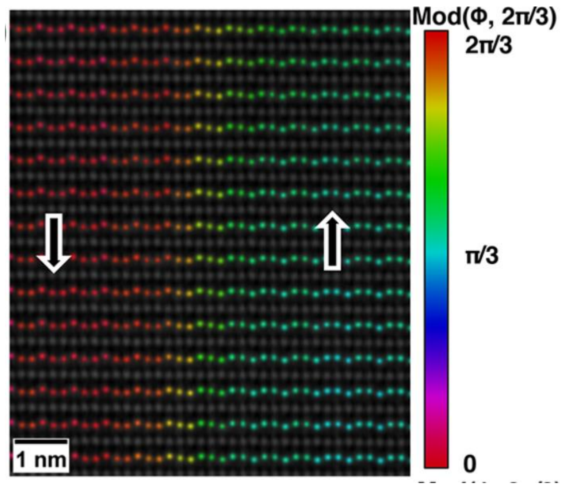




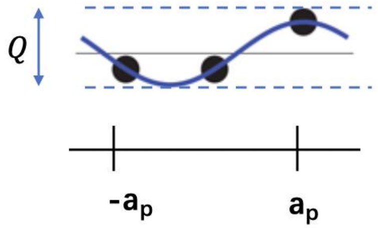
view from [1-10] direction
displacement of rare earth







when ϕ deviates from $\frac{n\pi}{3}$
near domain wall



2 dimension for plane

$$u(\boldsymbol{r_n}) = u_0 + Q_1 \cos \boldsymbol{q} \cdot \boldsymbol{r_n} + Q_2 sin\ \boldsymbol{q} \cdot \boldsymbol{r_n}$$

1 dimension for atom row （rare earth）

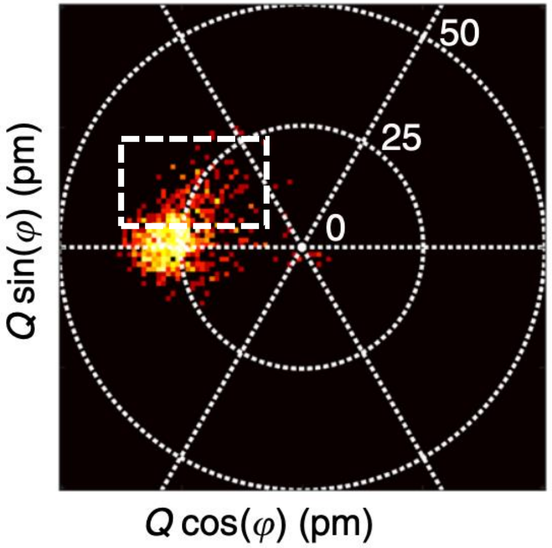
$$u(\mathrm{x}) = u_0 + Q\cos(qx - \phi)$$

given the position for three atoms (through quantitative
analysis of tem image—getting atom position in sub angstrom precision)

$x_1=-a_p$, y_1
$x_2=0$, y_2
$x_3=a_p$, y_3

$$\phi = \arctan\left(\frac{b}{b-1}\tan\left(\frac{qa_p}{2}\right)\right)$$

$$b = \frac{1}{2}\frac{y_1 - y_3}{y_2 - y_3} \quad q * 1.5a_p = \pi$$

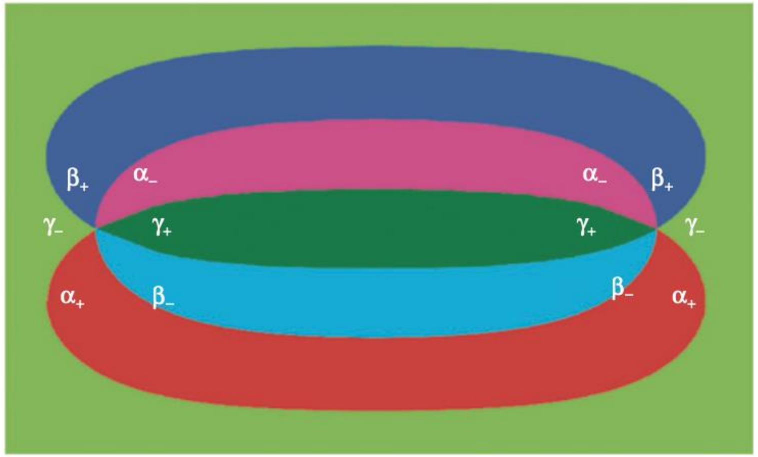


Topological stripe domain

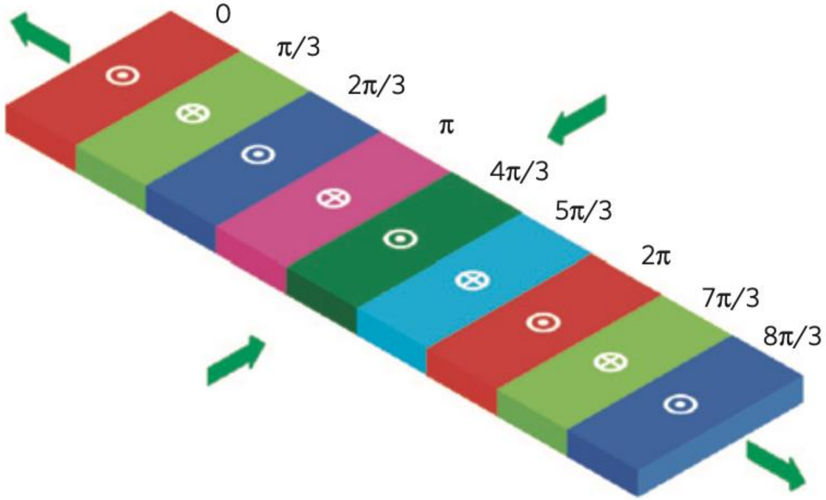
low-order coupling of inhomogeneous trimerization to strains

$$f_{strain} = -GQ^2[\,(u_{xx} - u_{yy})\partial_x\phi - 2u_{xy}\partial_y\phi]$$

u_{ij} *strain tensor*



vortex *anti-vortex*

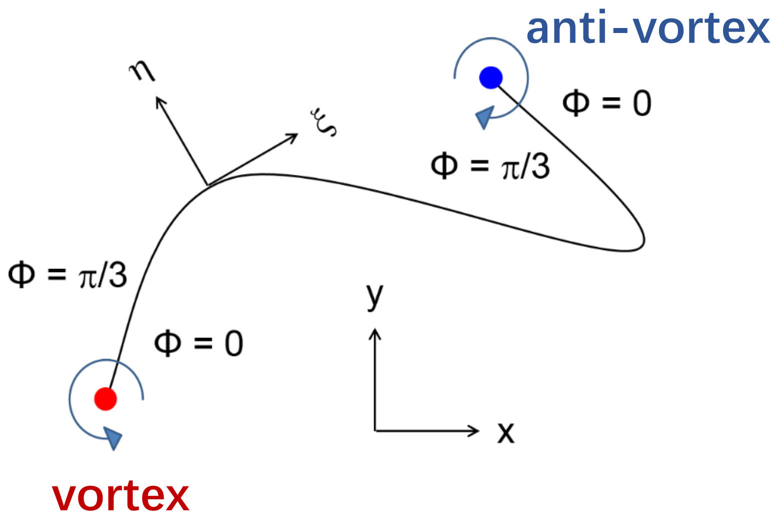


topological stripe domain

$$\Delta\phi = \frac{\pi}{3}$$

formation mechanism

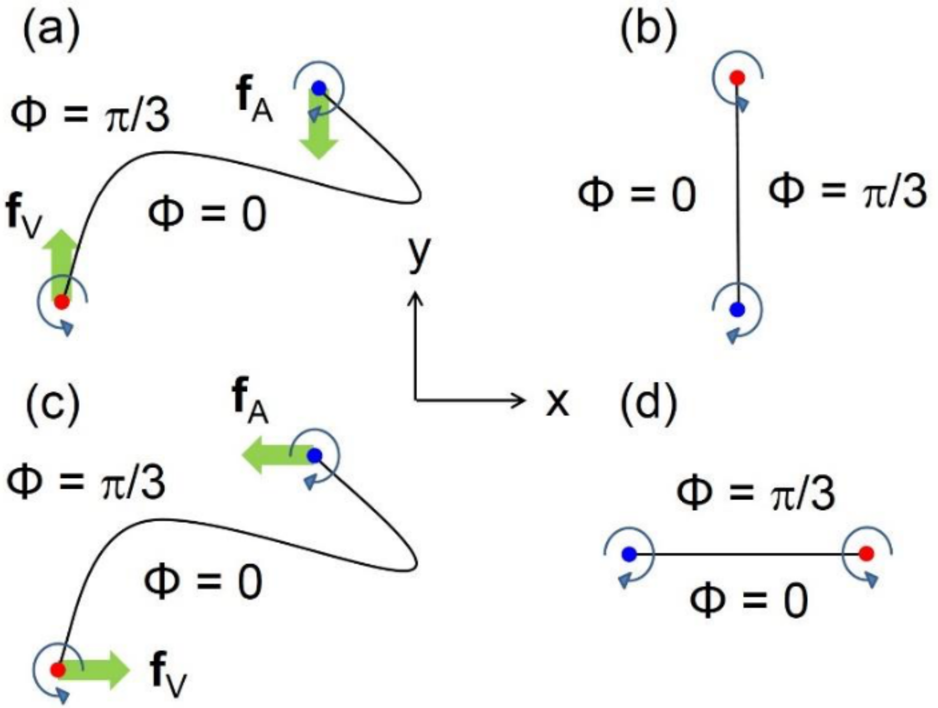
Magnus-type force between vortex and antivortex



$$\frac{\partial \phi}{\partial \eta} = \frac{\pi}{3}\delta(\eta)$$

$$f_{strain} = -GQ^2[(u_{xx} - u_{yy})]\partial_x \phi - 2u_{xy}\partial_y \phi$$

$$f_v = -f_A = GQ^2 h\frac{\pi}{3}(2u_{xy}, (u_{xx} - u_{yy}))$$



$\boldsymbol{u_{xy} = 0}$

$\boldsymbol{GQ^2(u_{xx} - u_{yy}) > 0}$

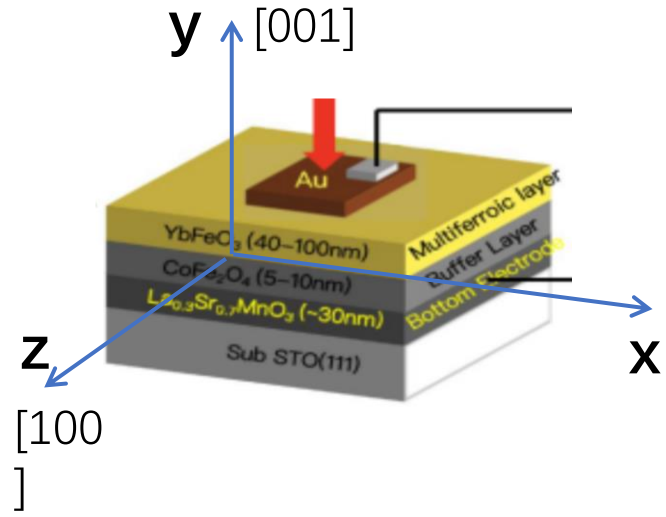
vertical stripe

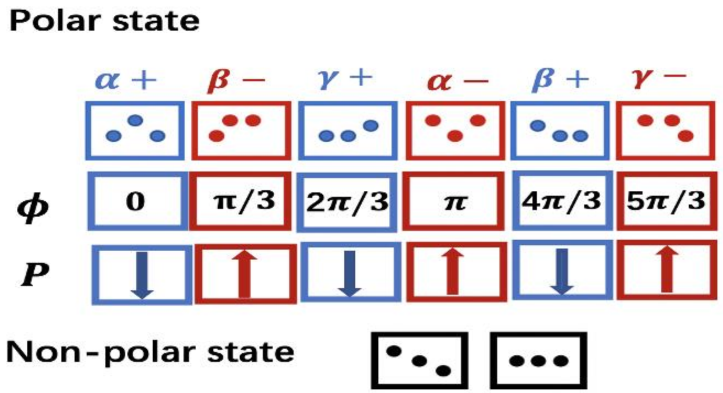
horizontal stripe

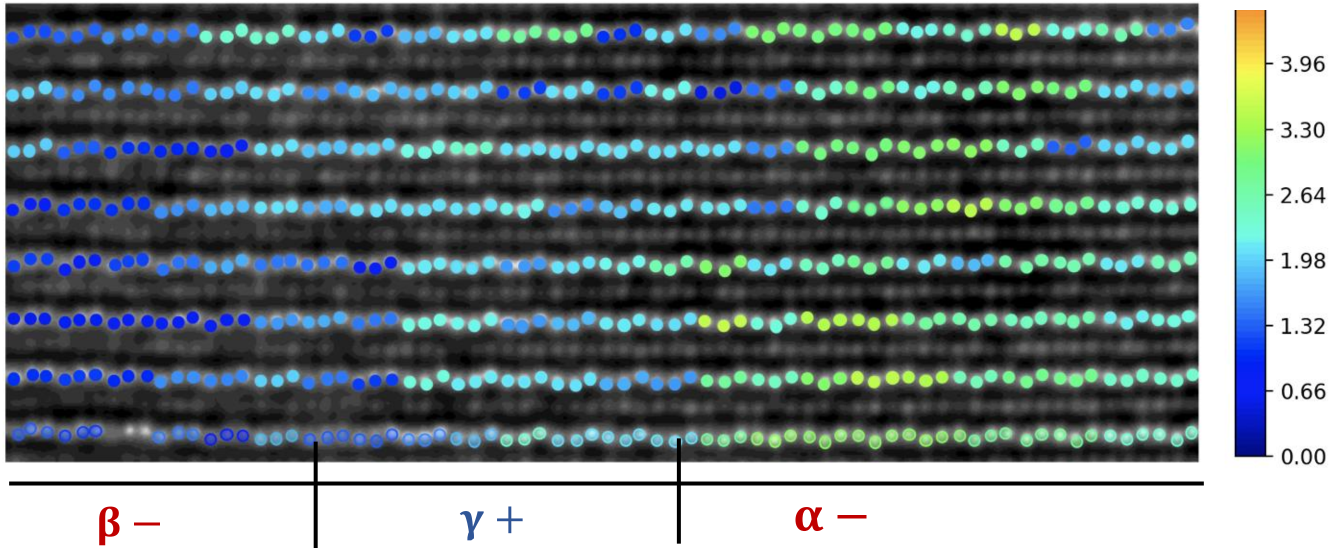
$\boldsymbol{u_{xx} - u_{yy} = 0}$

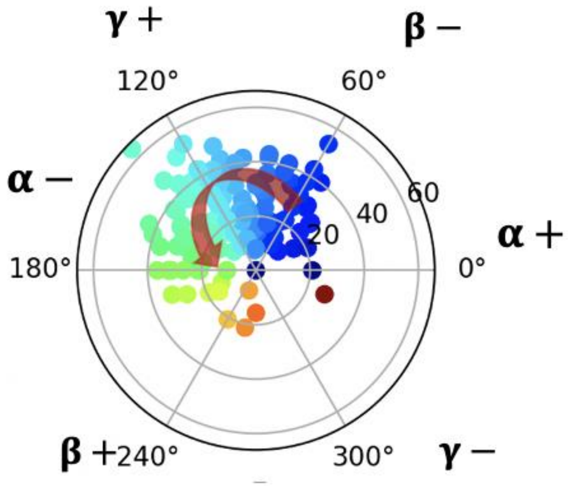
$\boldsymbol{GQ^2 u_{xy} > 0}$

Topological stripe domain
in h-$YbFeO_3$/CFO/LSMO film









Summary

1. **Inhomogeneous strain induced stripe domain in h-$YbFeO_3$/CFO/LSMO film**
2. **neighboring structural domains satisfy $\Delta\boldsymbol{\phi} = \frac{\boldsymbol{\pi}}{\mathbf{3}}$**

Reference

1. Nordlander, J., Campanini, M., Rossell, M.D. *et al.* The ultrathin limit of improper ferroelectricity. *Nat Commun* 10**,** 5591 (2019)
2. Megan E. Holtz .et al. Topological Defects in Hexagonal Manganites: Inner Structure and Emergent Electrostatics . Nano Lett17, 5883–5890 (2017)
3. Artyukhin, S., Delaney, K., Spaldin, N. *et al.* Landau theory of topological defects in multiferroic hexagonal manganites. *Nature Mater* 13**,** 42–49 (2014).
4. X. Wang, M. Mostovoy. et al. Unfolding of Vortices into Topological Stripes in a Multiferroic Material. Phys. Rev. Lett. 112, 247601(2014)