

Topological phase transitions in passive/active particles with chiral interactions

Department of Physics, Nagoya University
Takeshi Kawasaki

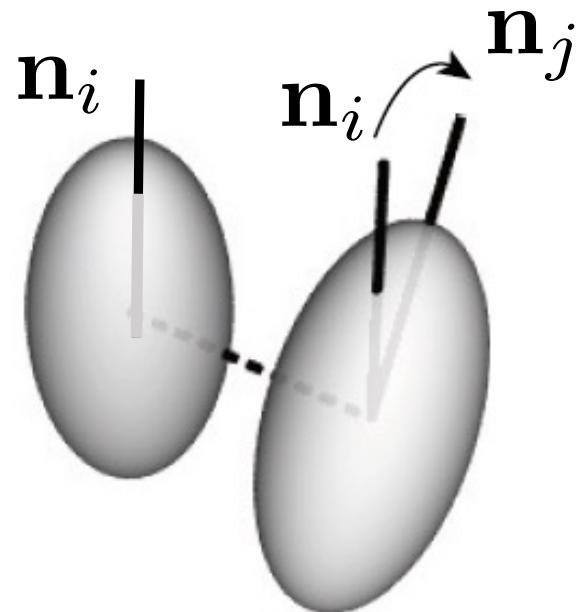
Collaboration with:
Kyohei Takae (Main player, U. Tokyo),
Arata Suzuki (Nagoya U.), Kunimasa Miyazaki (Nagoya U.)

Ref: K. Takae and T. K., PNAS 119, e2118492119 (2022)

Introduction: Chiral interactions

■ Chiral interactions:

- Resulting in a stable twist between neighbors for one direction.
- Widely appearing in both quantum and classical systems.



■ Examples:

- Quantum: Dzyaloshinskii-Moriya interaction in chiral magnets:

$$F_{\text{DM}} = \int d\mathbf{r} \ D [\mathbf{m} \cdot (\nabla \times \mathbf{m})], \quad \mathbf{m}: \text{magnetization.}$$

- Classical: Chiral steric interaction in cholesteric liquid crystal:

$$F_{2'} = \int d\mathbf{r} \ K_2' [\mathbf{n} \cdot (\nabla \times \mathbf{n})], \quad \mathbf{n}: \text{molecular orientation.}$$

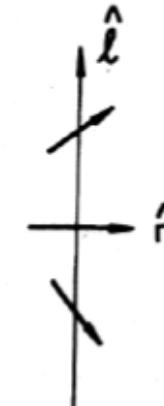
- Similar mathematical structure.

Introduction: Topological phases

■ In chiral interaction systems:

Topological structures (i.e., vortex, helix) are not just defects but stable as equilibrium phases.
➤ **Topological phases**

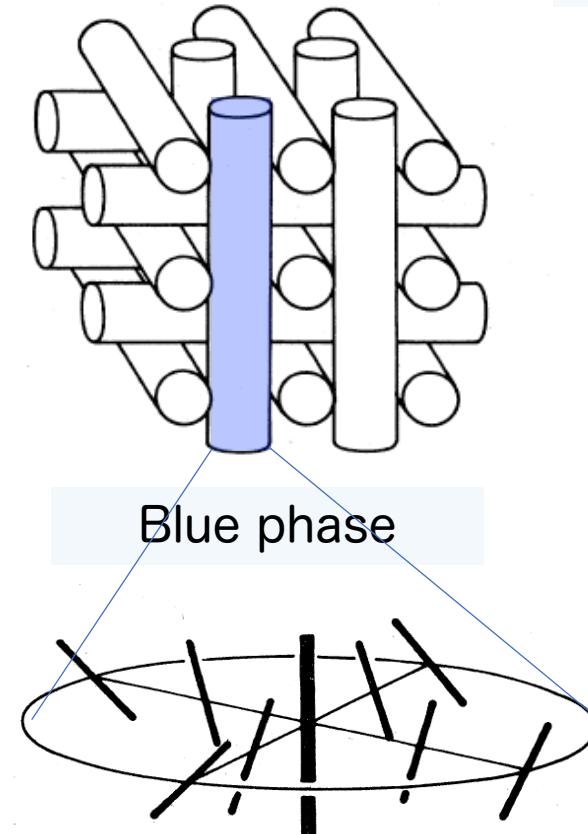
■ Topological phases in CE4 chiral liquid crystal:



Cholesteric phase

➤ Helical structure

D. C. Wright and N. D. Mermin, Rev. Mod. Phys. 61, 385 (1989).

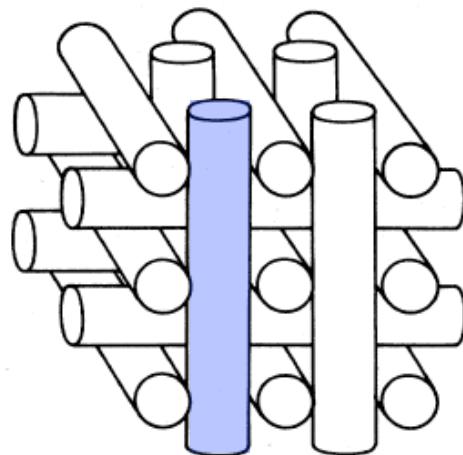


➤ Double twist cylinder

Introduction: Topological phases of cholesteric liquid crystals under thin-film constraints

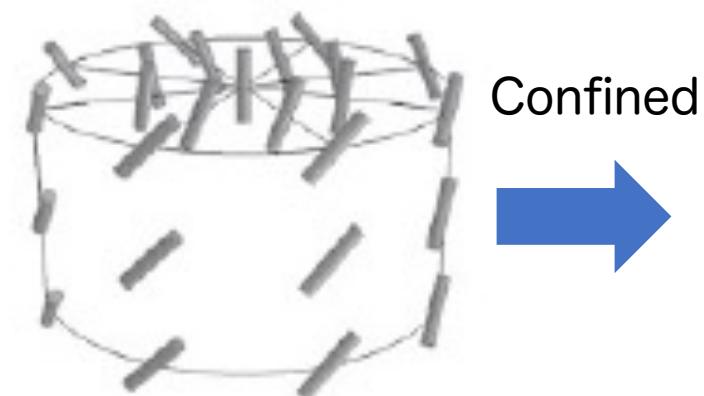
■ Cholesteric liquid crystal under thin film constraint:

➤ Bulk cholesteric blue phase



Blue phase

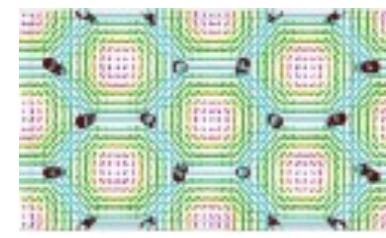
➤ Blue phase confined in thin films



Double twist cylinder



Half-skyrmion (melon)



GL theory



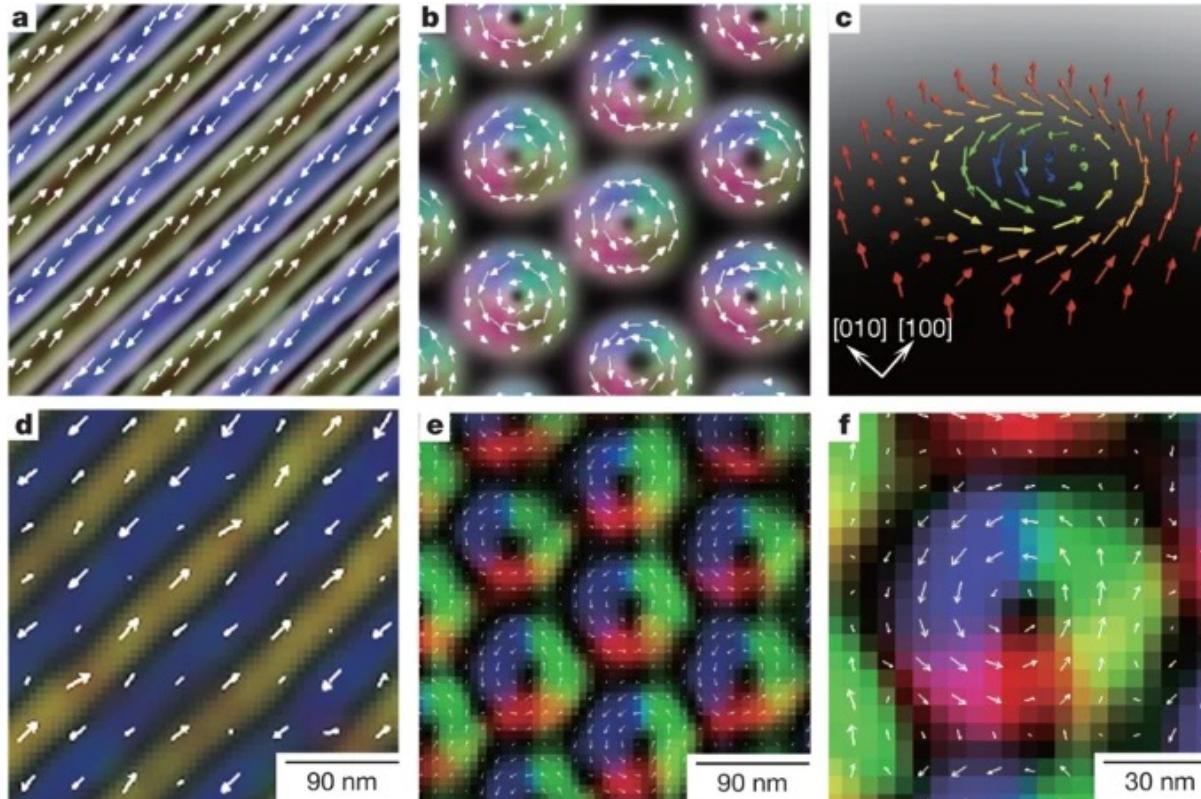
Experiment

J. Fukuda and S. Žumer, Nat. Commn. 2, 1 (2011).
A. Nych, et al., Nat. Phys. 13, 1215 (2017).
D. Foster, et al., Nat. Phys. 15, 7 (2019).

Introduction: Topological phases in chiral magnets

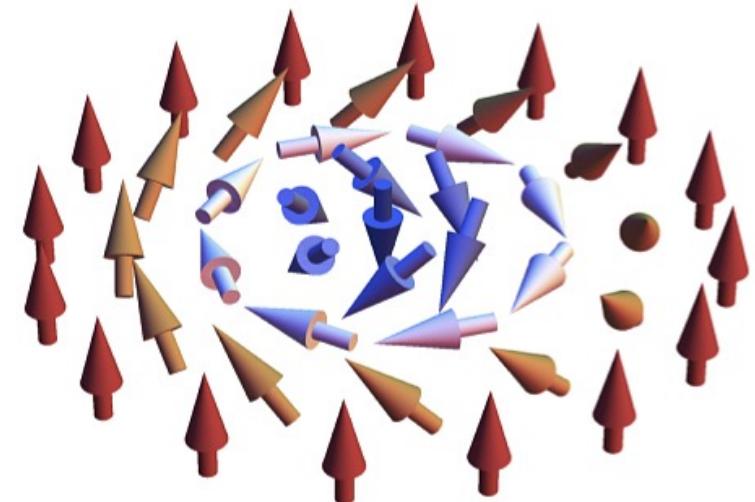
■ Topological phases in confined chiral magnets $\text{Fe}_{0.5}\text{Co}_{0.5}\text{Si}$

Simulations



Helical phase
(low temperature, zero
magnetic field)

Skyrmion phase
(low temperature, with
magnetic field)



https://www.riken.jp/press/2014/20140127_1/

X. Z. Yu, Y. Onose, N. Kanazawa, J. H. Park, J. H. Han, Y. Matsui, N. Nagaosa, and Y. Tokura, Nature 465, 901 (2010).

Problem statement

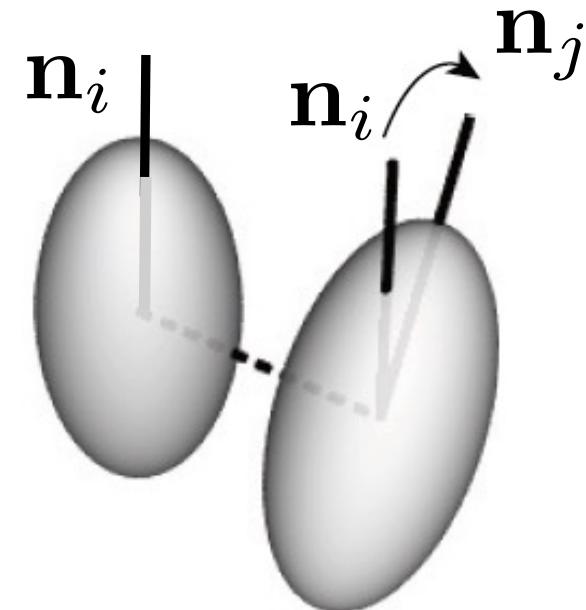
- The mathematical similarity in the energetic forms of quantum- and classical-chiral interaction systems.
 - With chiral interactions, similar quantum-like topological phases should be observed in a variety of soft-matter systems.
 - Despite this possibility, such phases have not been extensively studied except in cholesteric liquid crystals.
- The reason for this lack:
 - Microscopic models, such as molecular dynamics, have rarely been developed.

Purpose

- Construct a simple/general MD simulation model with **chiral interactions**.
- Explore exotic topological phases for wide-range of soft matter systems.

Model and numerical methods (EoMs)

- Model:
 - Anisotropic particle system considering chirality.
- Numerical Methods
 - Classical molecular dynamics simulations



Translation:

$$m_\alpha \ddot{\mathbf{r}}_i = -\frac{\partial U}{\partial \mathbf{r}_i}$$

Rotation:

$$I_1 \mathbf{n}_i \times \ddot{\mathbf{n}}_i = -\mathbf{n}_i \times \frac{\partial U}{\partial \mathbf{n}_i}$$

K. Takae and T. K., PNAS 119, e2118492119 (2022).

Model and numerical methods (interactions)

- Particle interaction potential (constructed in this study).

$$U = \sum_{i < j} 4\epsilon (1 + A_{ij} + B_{ij}) \left(\frac{\sigma}{r_{ij}} \right)^{12} + U_{\text{wall}}$$

- Anisotropy of molecular shape

$$A_{ij} = \eta [(\mathbf{n}_i \cdot \hat{\mathbf{r}}_{ij})^2 + (\mathbf{n}_j \cdot \hat{\mathbf{r}}_{ij})^2] \quad \frac{a_\ell}{a_S} = (1 + 2\eta)^{\frac{1}{6}} \sim 1.1$$

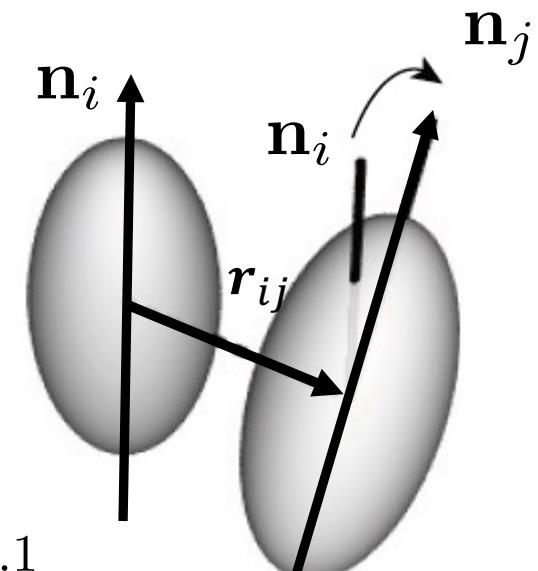
- Twist interactions between molecules

$$B_{ij} = \frac{K_2}{2} [(\mathbf{n}_i \cdot \mathbf{n}_j)(\mathbf{n}_i \times \mathbf{n}_j) \cdot \hat{\mathbf{r}}_{ij} - q_0]^2$$

- Wall: repulsive

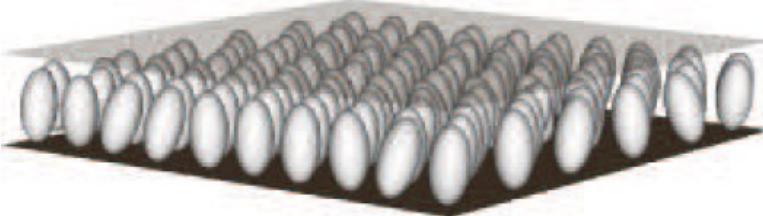
$$U_{\text{wall}} = \sum_i \epsilon \left[\left(\sigma/z_i \right)^{12} + \left(\sigma / (L_z - z_i) \right)^{12} \right]$$

K. Takae and T. K., PNAS 119, e2118492119 (2022).

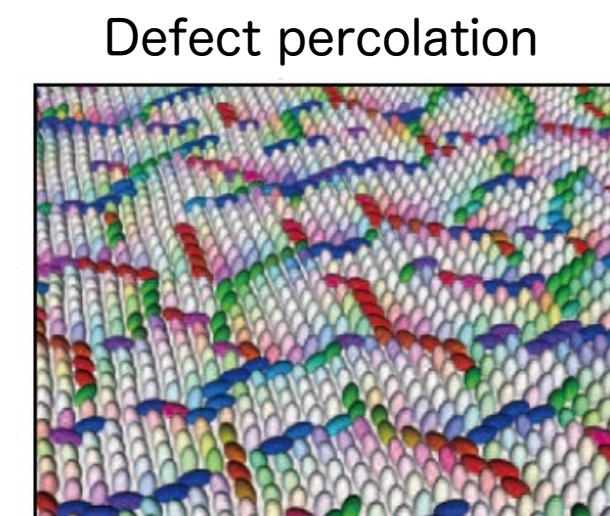
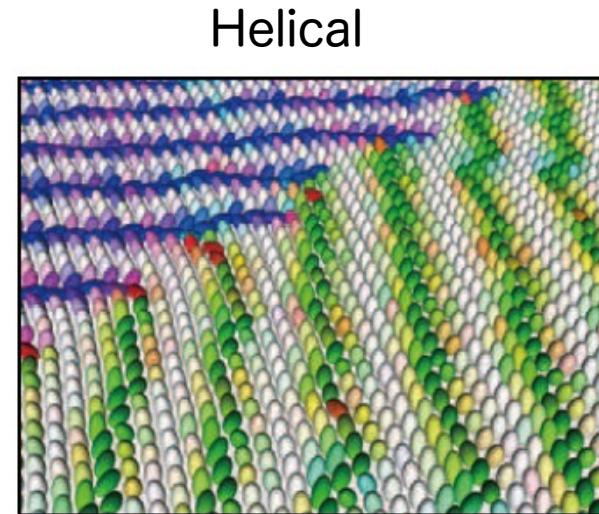
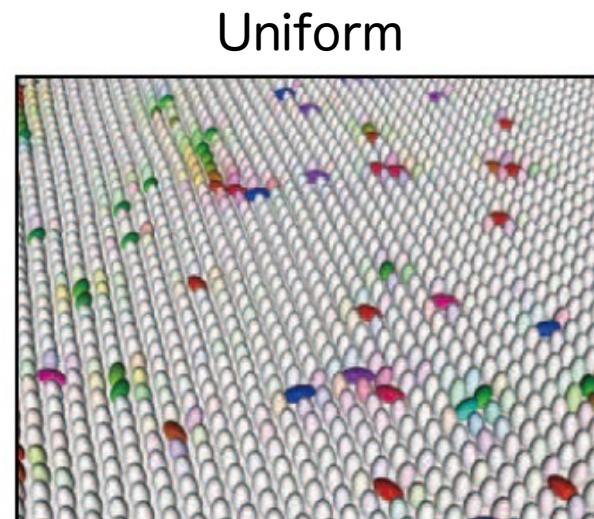
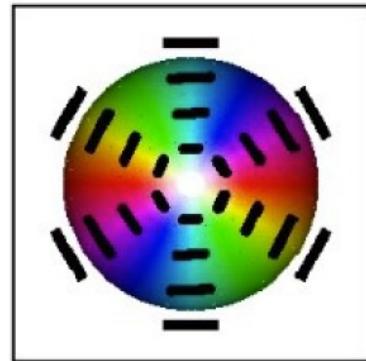


Results: Various topological phases obtained with this model

Confine the particles in quasi-two-dimensional space **at low temperature and high density.**



Colors: orientation of the particles



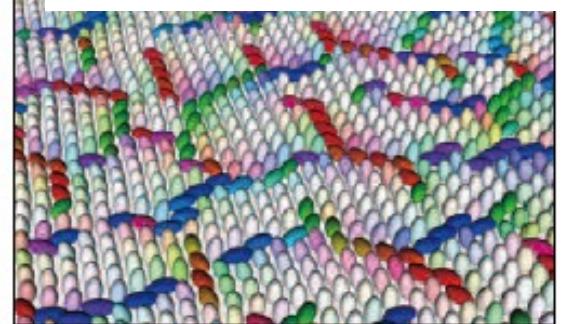
- Control of material parameters (q_0 , K_2) in:

$$B_{ij} = \frac{K_2}{2} [(\mathbf{n}_i \cdot \mathbf{n}_j)(\mathbf{n}_i \times \mathbf{n}_j) \cdot \hat{\mathbf{r}}_{ij} - q_0]^2$$

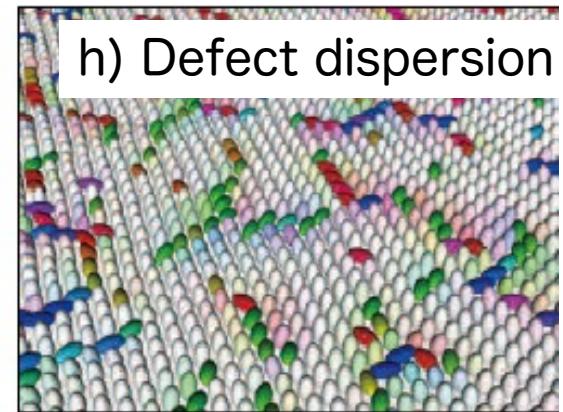
K. Takae and T. K., PNAS 119, e2118492119 (2022).

Results: Equilibrium phase diagram (change in material parameters)

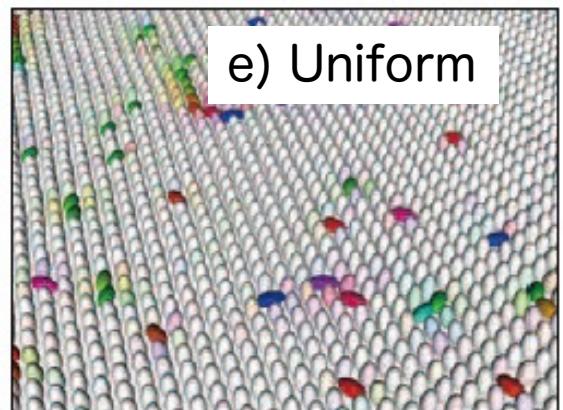
i) Defect percolation



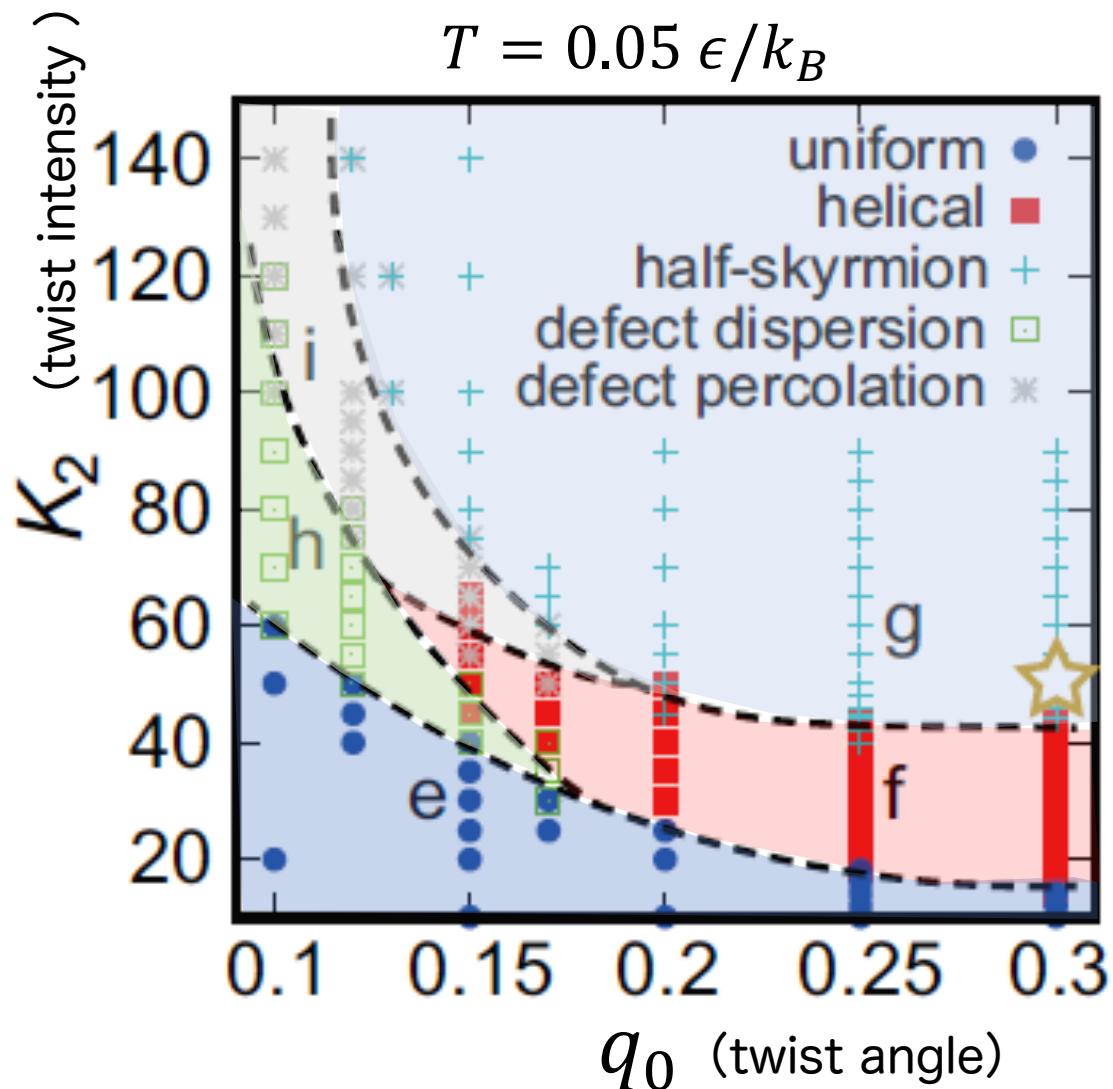
h) Defect dispersion



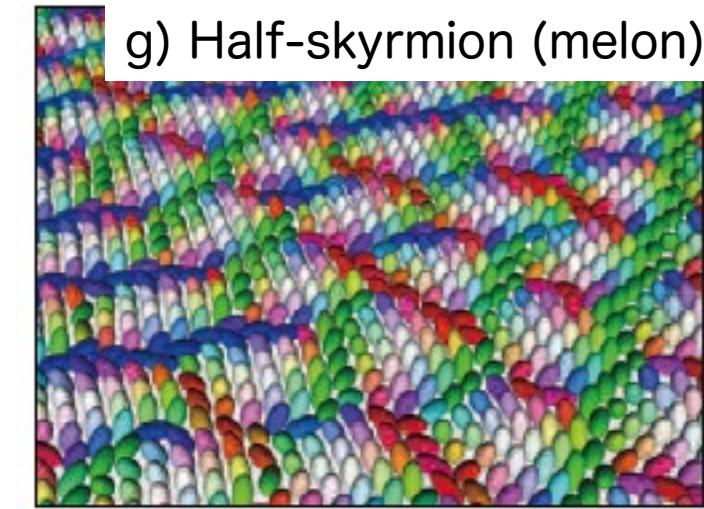
e) Uniform



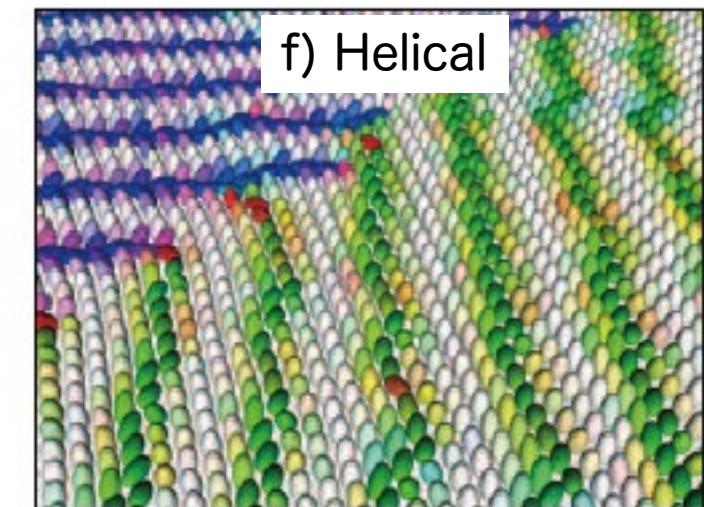
$T = 0.05 \epsilon/k_B$



g) Half-skyrmion (melon)

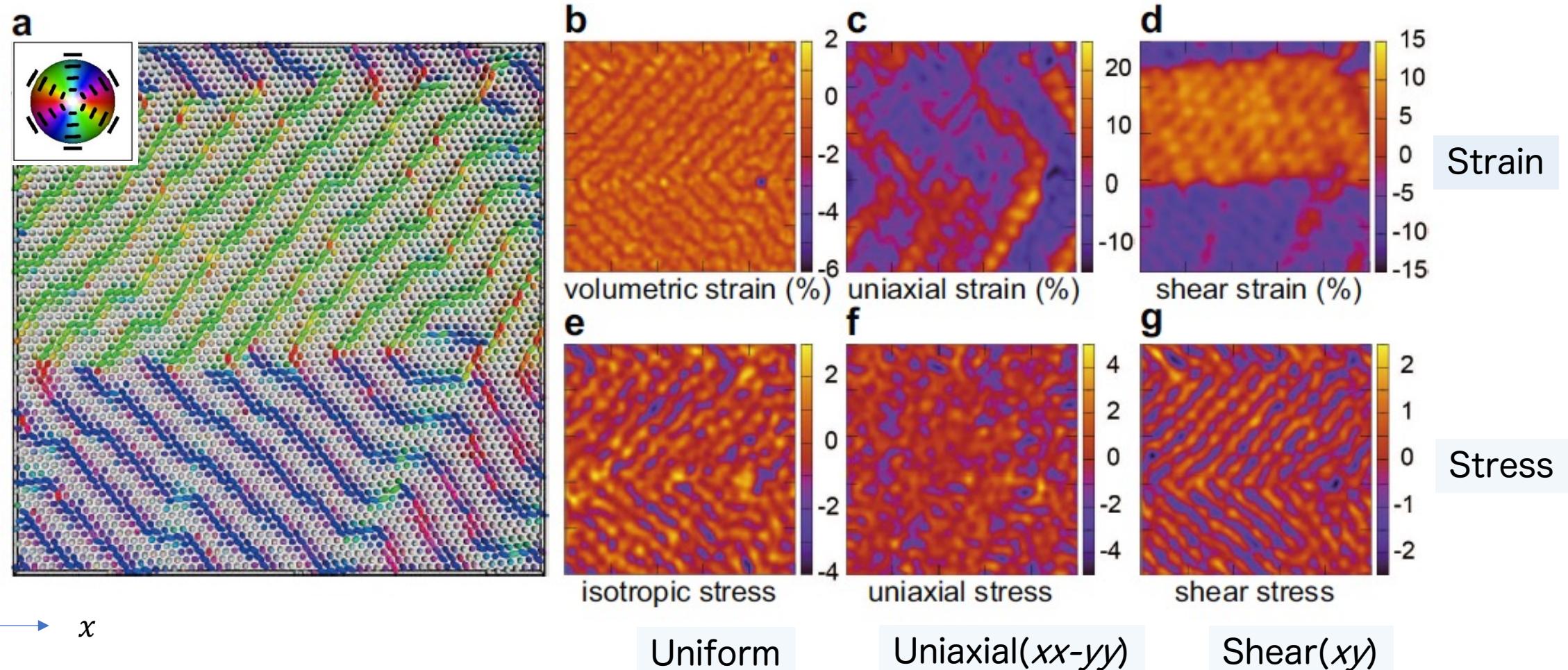


f) Helical

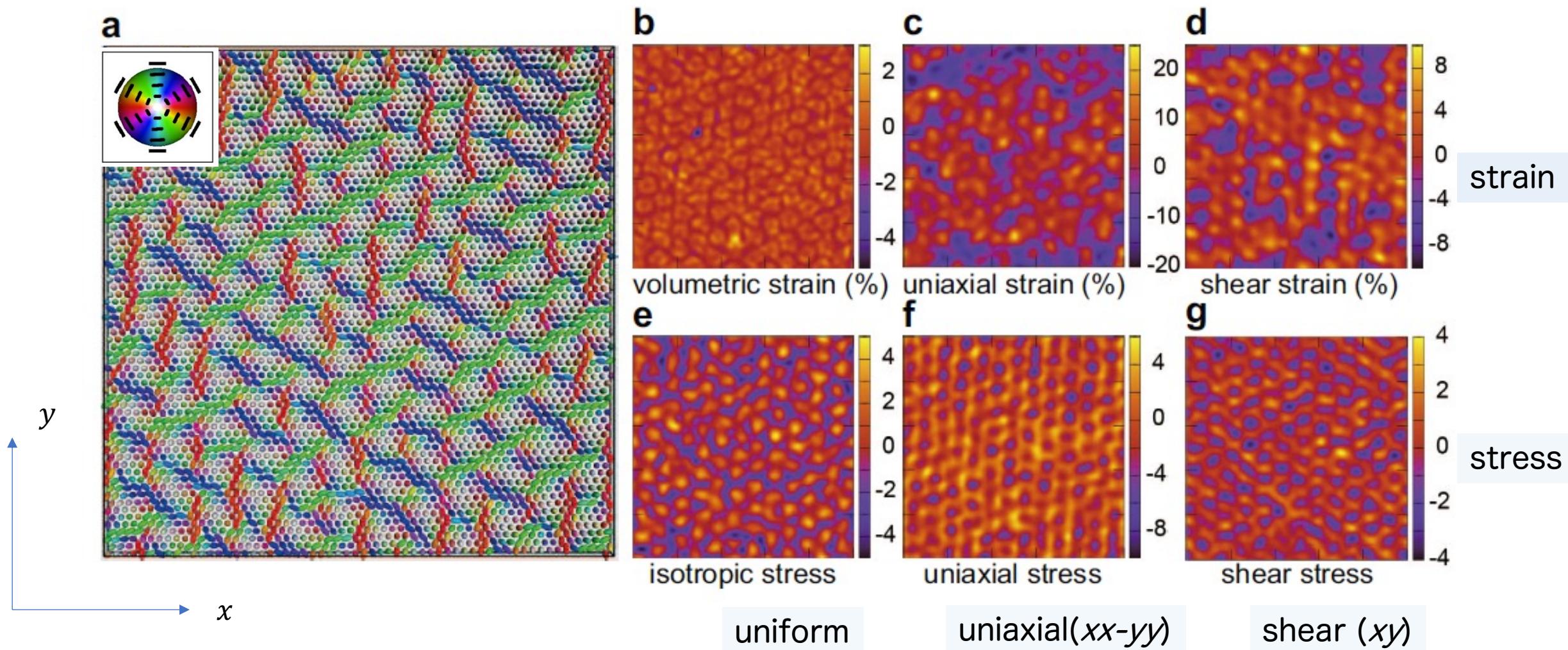


Results: Local elastic fields (Helical phase)

Measuring local strain and stress fields: large anisotropic strains occur (c,d), domains are formed to resolve the resulting stresses, and stresses are relaxed (f,g).



Results: Local elastic fields (Half skyrmion phase)

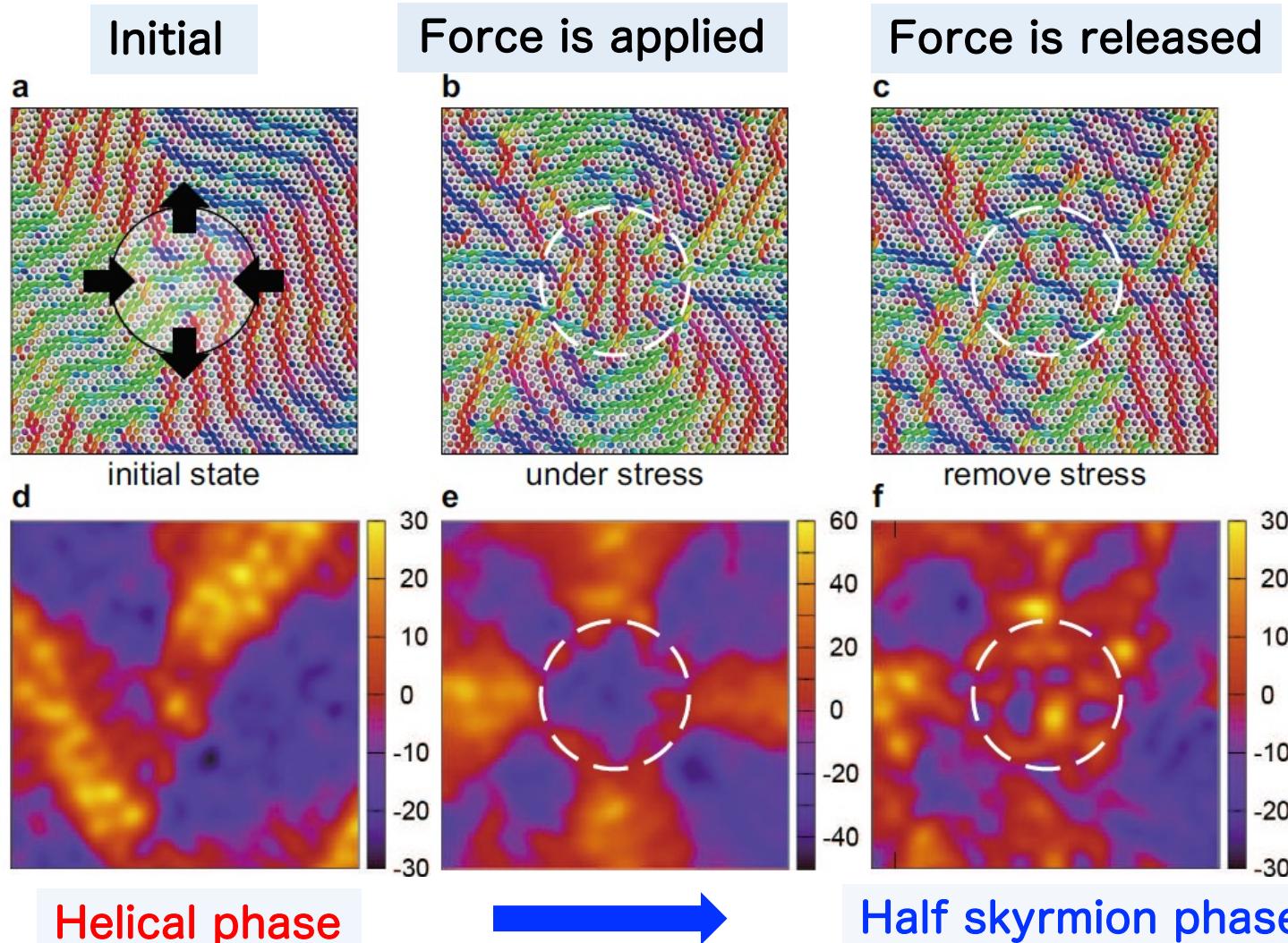


- Characteristic elastic field emerges due to topological phase transition
 - “*Emergent elastic field*”

Results : Control of emergent elastic field

- Localized force applied to helical phase (black and white circles)
- The area, the force is applied changes to the half-skyrmion phase.

Particle orientation



■ The application of an external force can change the structure of the system, and control its physical properties.

■ Such behaviour could be significant in applications.

Summary

Our system

	Chiral magnets	Cholesteric liquid crystal	Chiral molecular crystals
Quantum/Classical	Quantum	Classical	Classical
Chiral interactions	Dzyaloshinskii-Moriya	Twist elasticity	Twist elasticity
Characteristic phases	Helical, Skyrmiion phase	Helical, Skyrmiion, Blue phase	Helical, Half-skyrmion phase
Emergent fields	Emergent electro-magnetic field	Nematic director fields	Emergent elastic field
Size of vortexes	5-100nm	100 ~ nm	A few times of the particles (molecule: nm,colloid: μm)
Liquid-solid transition of Skrmions	BKTHNY	N/A	BKTHNY

Our findings (in red)

- The feature of the chiral softmatter system:
 - The topology and elastic field are strongly coupled due to the steric repulsion !

K. Takae and T. K., PNAS 119 e2118492119 (2022)

Perspective: Application to active matter

■ Active Brownian particles (ABP):

$$m\ddot{\mathbf{r}}_i = -\zeta_T \dot{\mathbf{r}}_i + f_0 \mathbf{n}_i - \partial_{\mathbf{r}_i} (U + U^{\text{wall}}) + \xi_i^T,$$

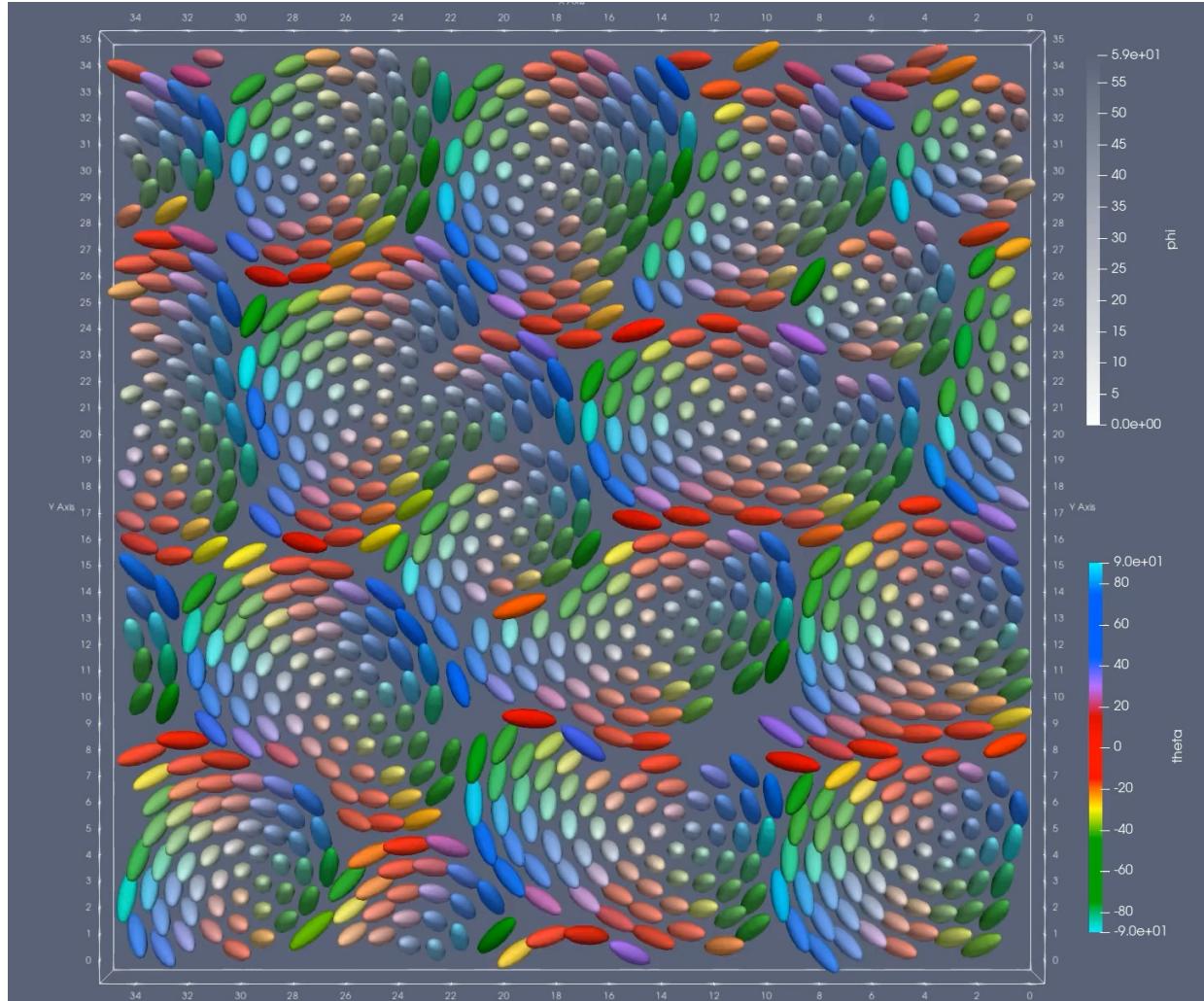
$$I(\mathbf{n}_i \times \dot{\mathbf{n}}_i) = -\zeta_R \mathbf{n}_i \times \dot{\mathbf{n}}_i - \mathbf{n}_i \times \partial_{\mathbf{n}_i} (U + U^{\text{wall}}) + \xi_i^R,$$

$$\langle \xi_i^\alpha \xi_j^\alpha \rangle = 2k_B T \xi_\alpha \delta_{ij} \mathbf{1} \quad (\alpha \in T \text{ or } R).$$

Achiral ABP + Chiral interactions

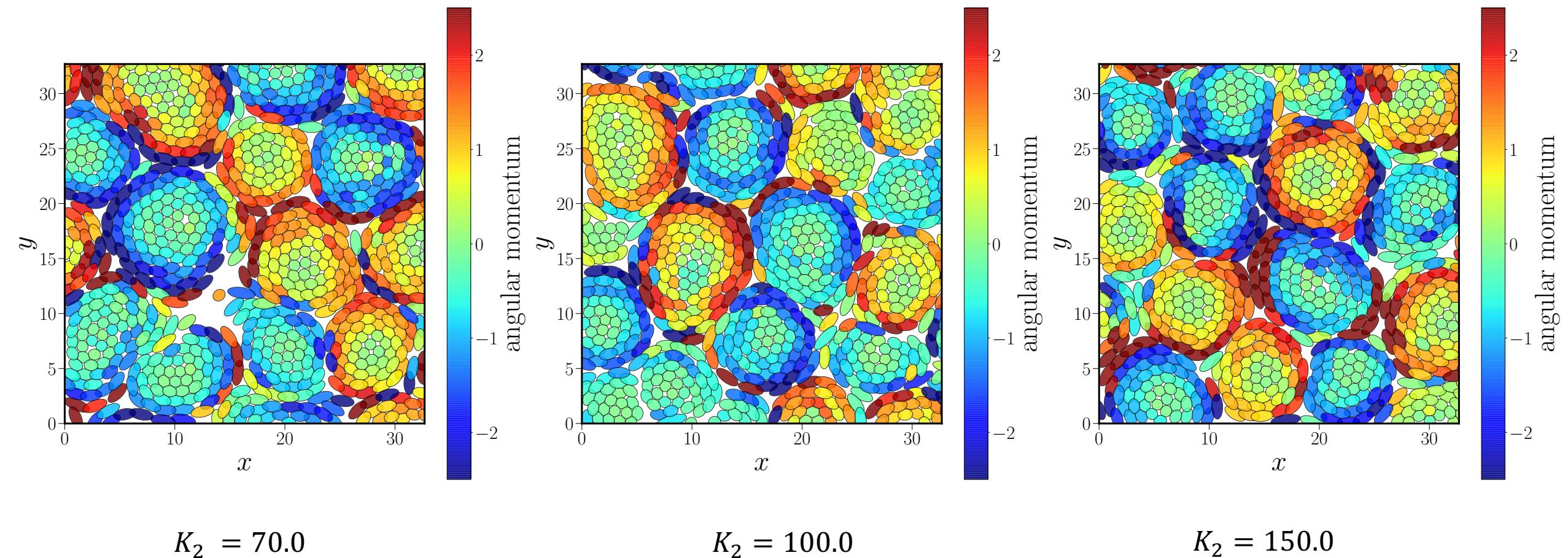


Whirling half-skyrmions!



(Q) Edge current? Experimental applications? …etc

Appendix: Whirling half-skyrmions



$$K_2 = 70.0$$

$$K_2 = 100.0$$

$$K_2 = 150.0$$