Kavli IPMU - RIKEN iTHES - Osaka TSRP Symposium

"Frontiers of Theoretical Science - MATTER, LIFE and COSMOS -"

Vortex loops in hexagonal rare-earth manganites ($RMnO_3$) and the Kibble-Zurek mechanism

(to appear in Nature Physics)

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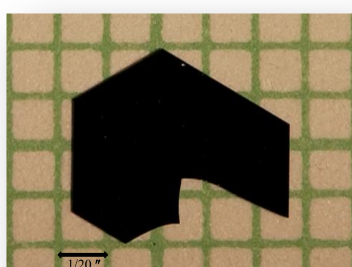
Experiments : S.-W. Cheong group & V. Kiryukhin group

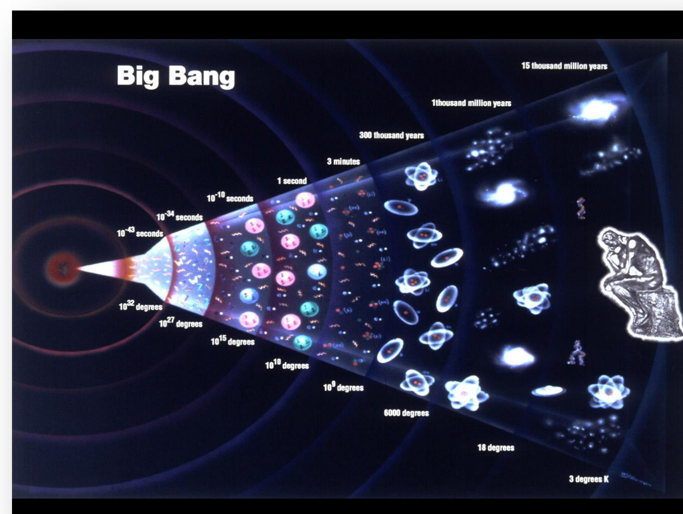
Los Alamos NATIONAL LABORATORY EST. 1943

The State University of New Jersey Rutgers Department of Physics and Astronomy

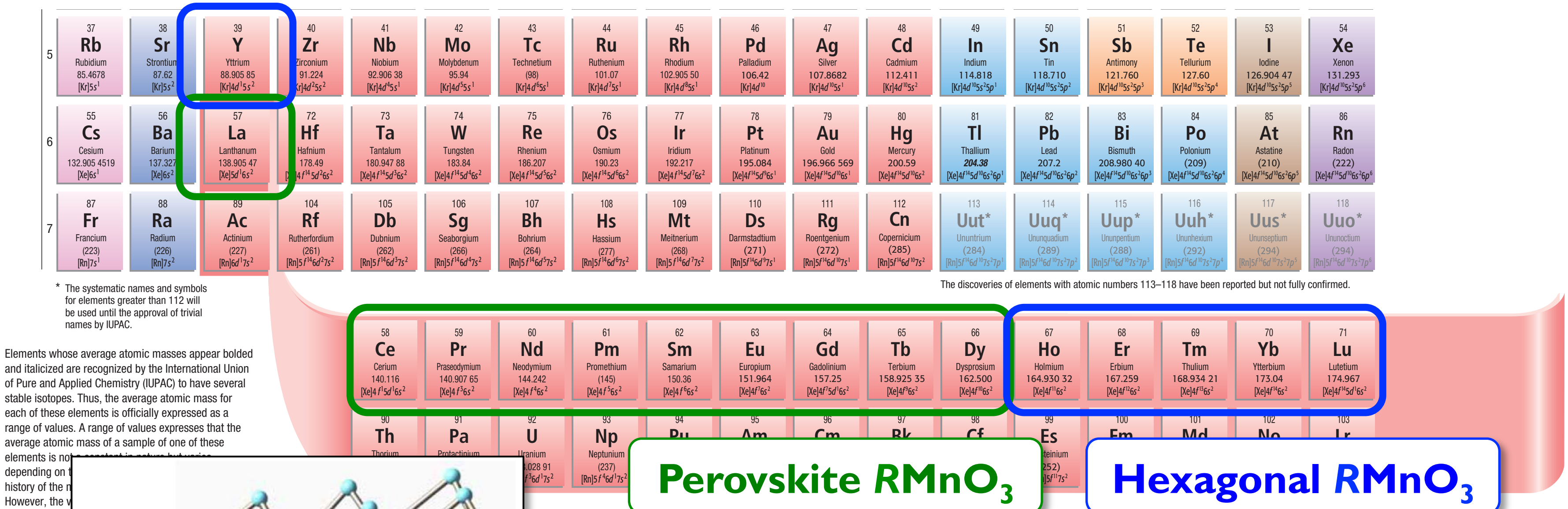
Outline

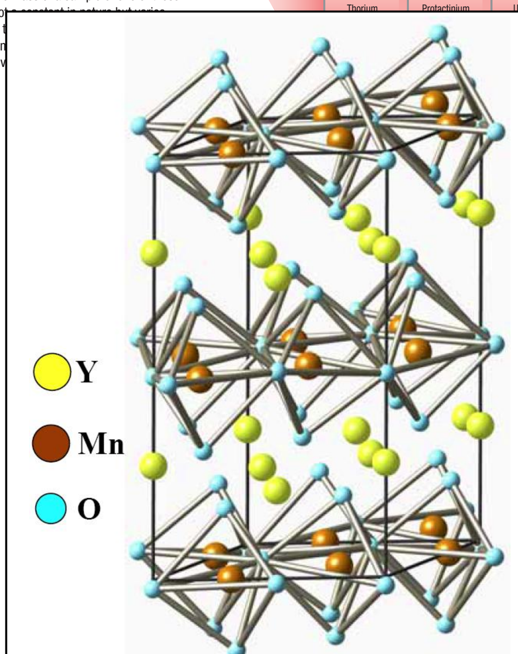
- Hexagonal rare-earth manganites ($RMnO_3$) and the "trimerization" (structural transition) inducing ferroelectricity
- Visualization of frozen vortex loops
- Theoretical modeling with a 6-state "clock spin" (Z_6) model in 3D
  - Emergent symmetry at the critical point : $Z_6 \rightarrow U(1)$
  - Dual (vortex-loop) description of the phase transition
- Comparison with the Kibble-Zurek theory





As R (rare earth) of $RMnO_3$, one may choose …

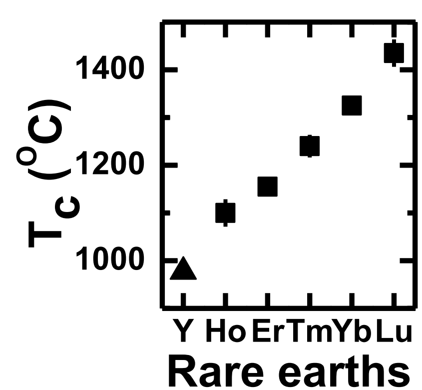




Common properties

- Ferroelectric insulators
- T_c > ~1300 K
- T_N ~ 100 K (*)

FE transition T



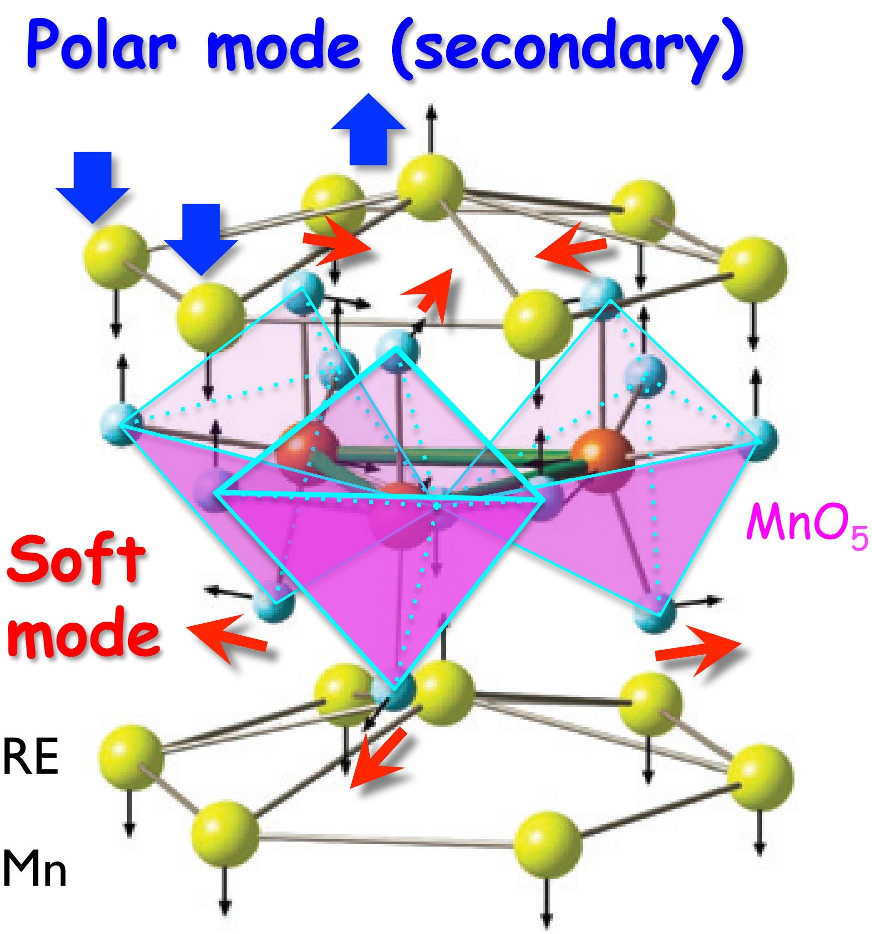
(* We are not concerned about magnetism in this talk)

Trimerization with Z_6 symmetry breaking

Buckling of MnO_5 polyhedra accompanied by displacements of rare earth ions

→ **Ferroelectricity**

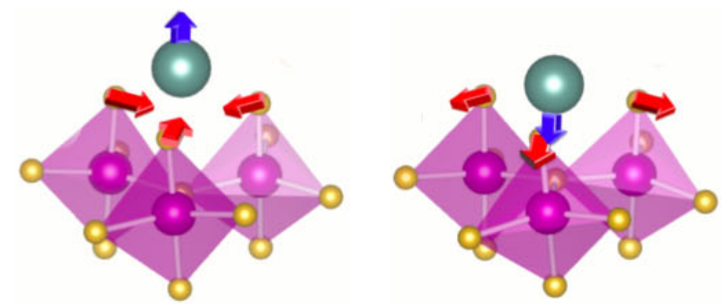
Bas B. Van Aken, et al., Nature 2004



RE

Mn

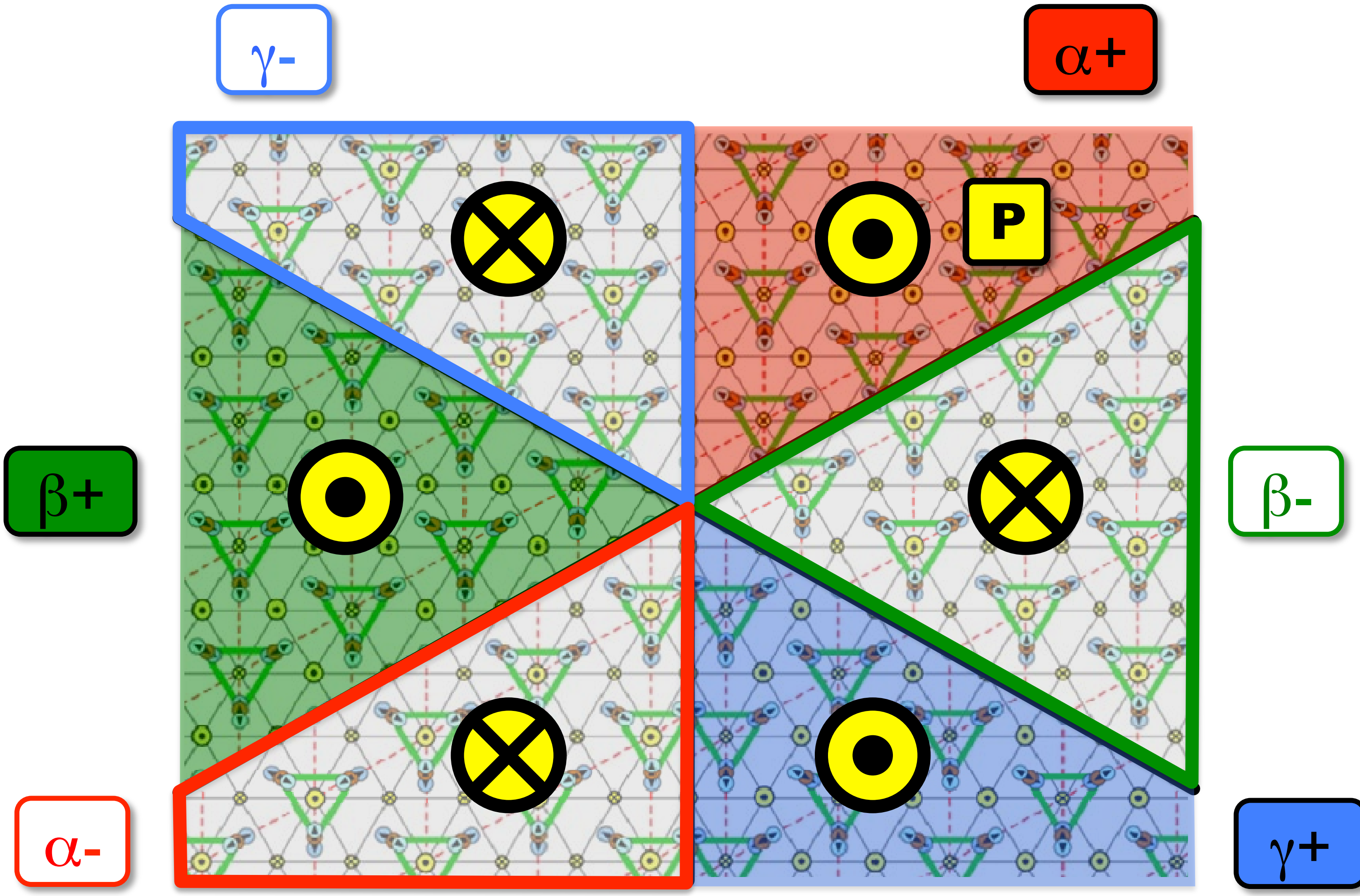
O



6 domain types

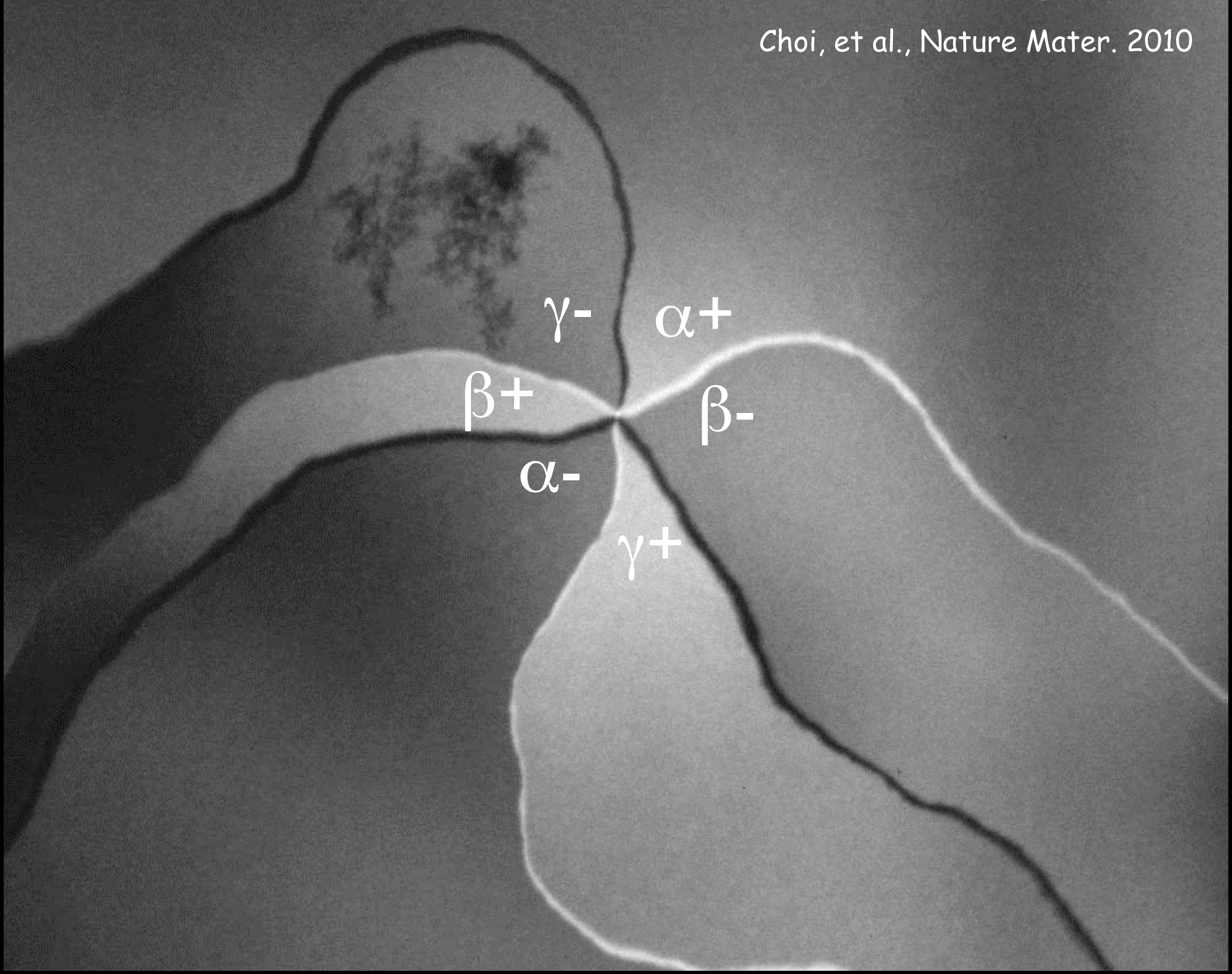
$$Z_3 \times Z_2 = Z_6 \qquad \alpha+, \alpha-, \beta+, \beta-, \gamma+, \gamma-$$

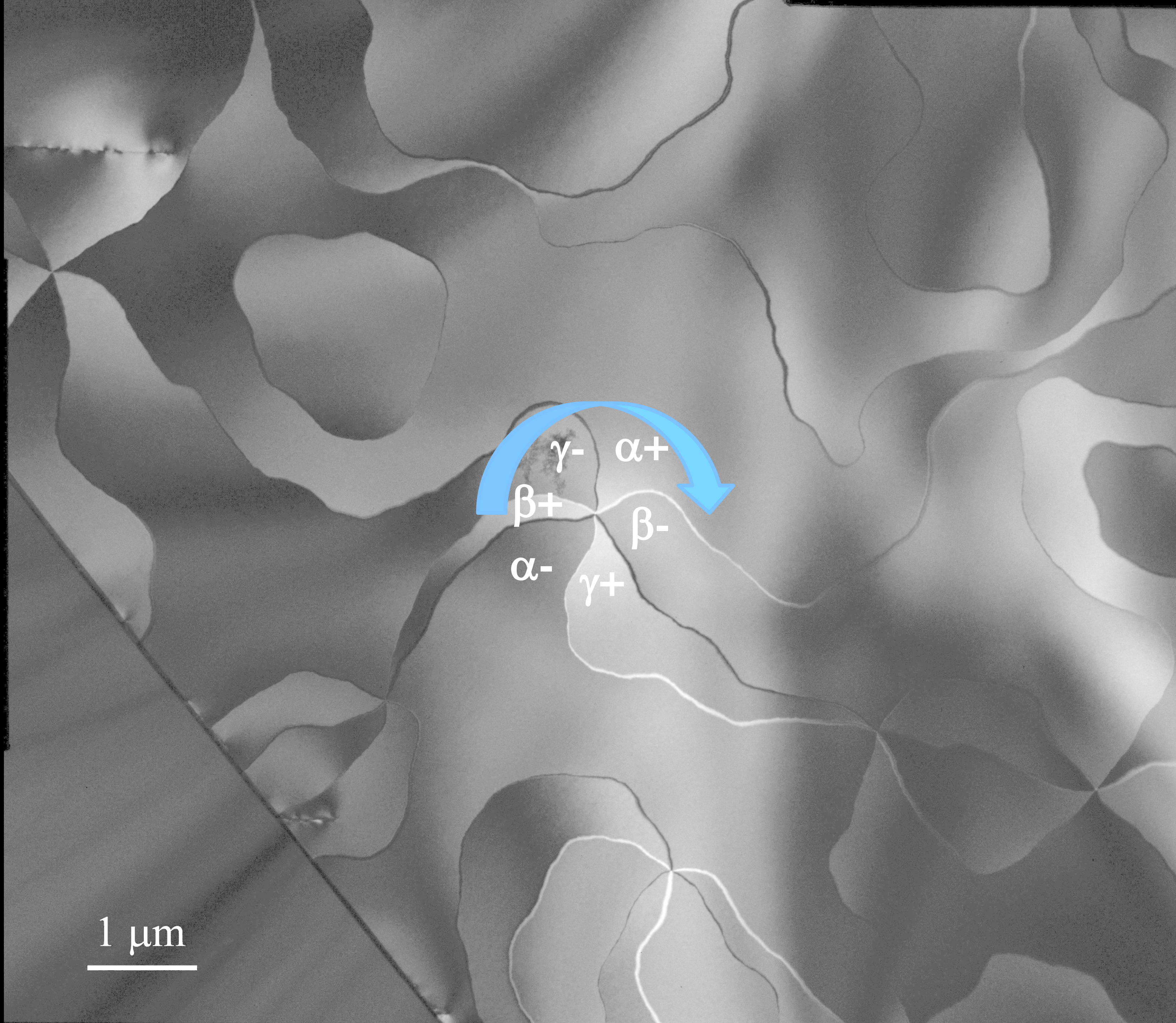
Vortex

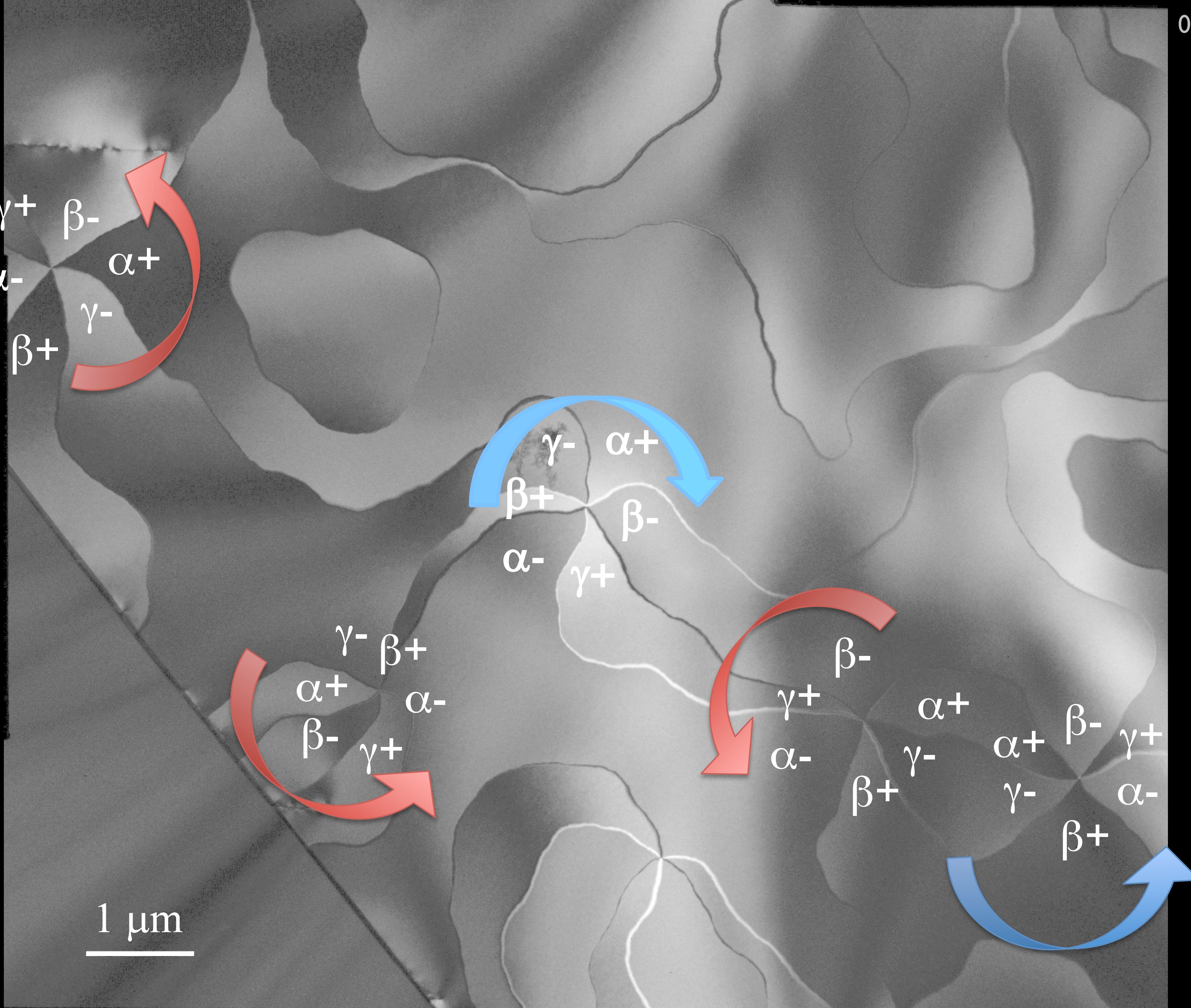


(The other types of domain walls appear to be energetically unfavorable)

TEM dark-field with (1-31) peak ($P6_3cm$)




γ-
α+
β+
β-
α-
γ+
1 μm


γ+ β-
α+
α-
γ-
β+
γ- α+
β+
β-
α-
γ+
γ- β+
α+
α-
β-
γ+
β-
γ+
α+
α-
γ-
β+
β-
α+
γ+
γ-
α-
β+
1 μm

Six-state "clock spin" (Z_6) model in 3D

$$\theta_i = \frac{n\pi}{3} \quad n = 0, 1, 2, 3, 4, 5$$

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \cos\left(\theta_i - \theta_j\right) - J' \sum_{\langle\langle kl \rangle\rangle} \cos\left(\theta_k - \theta_l\right)$$

intra-layer **inter-layer**

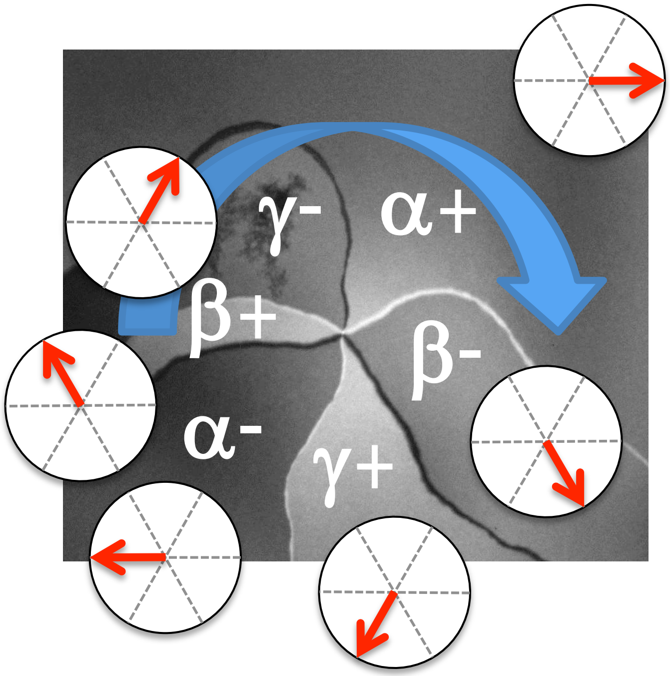
Natural model to explain the observed vortex structure

- Trimerization pattern (α, β, γ)

$$\mathbf{T}_i = (\cos 2\theta_i, \sin 2\theta_i)$$

- Electric polarization

$$\mathbf{P}_i = (\cos 3\theta_i, \sin 3\theta_i)\,\hat{z}$$



$Z_6 \rightarrow U(1)$

The Z_6 anisotropy is "dangerously irrelevant" in 3D

Blankshtein et al., PRB 1984
Oshikawa, PRB 2000

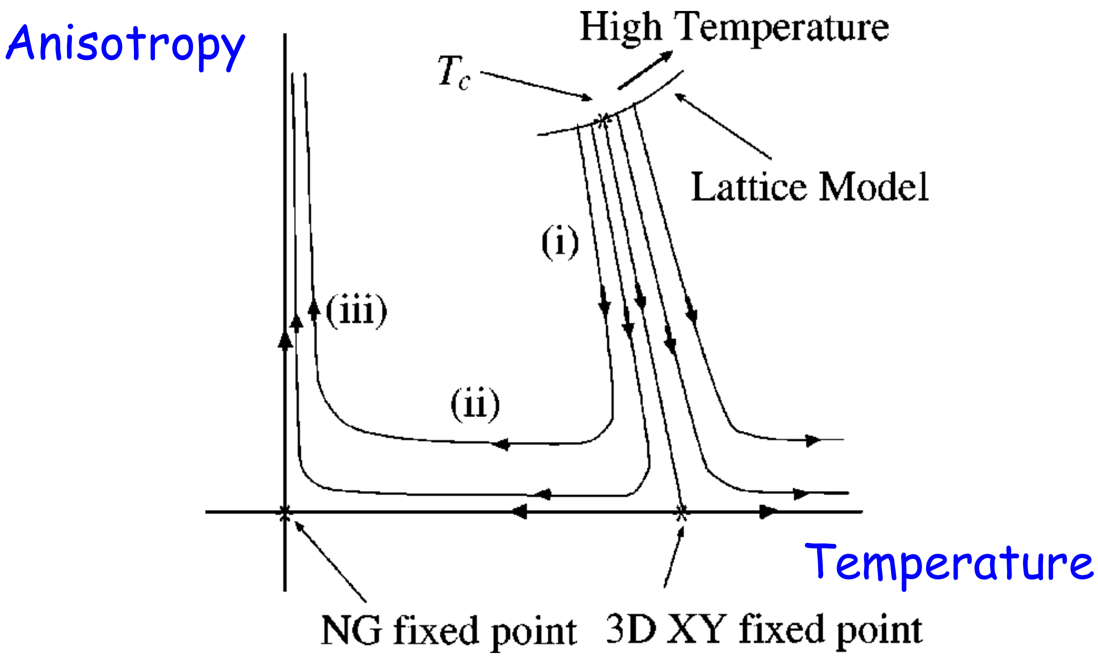
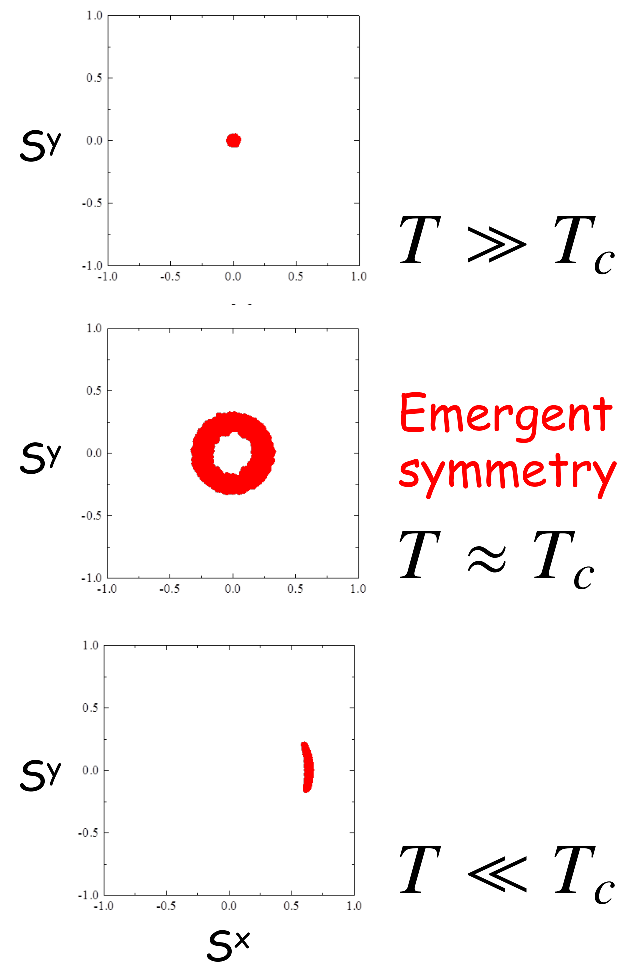
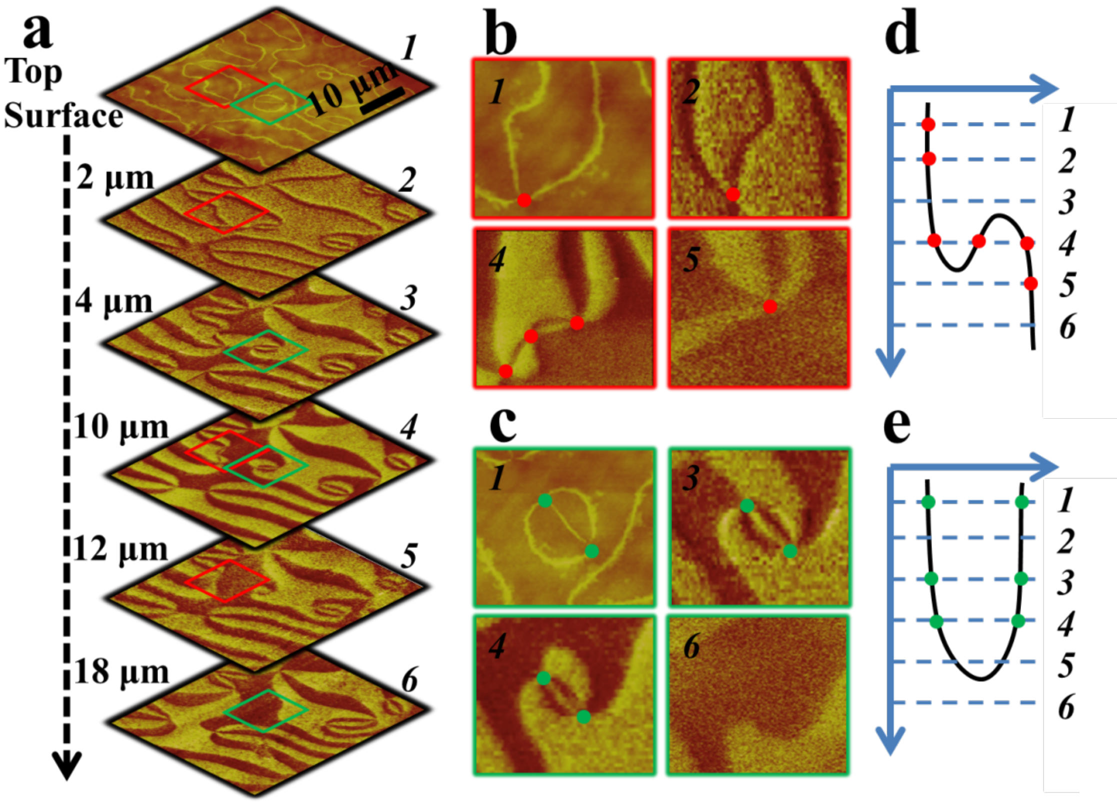


FIG. 1. The RG flow diagram of the Z_n models, projected onto the two-dimensional parameter space spanned by u and λ_n. The Z_n perturbation λ_n is irrelevant at the 3D XY fixed point, but is relevant at the NG fixed point. For T slightly less than T_c, the RG flow is divided into the three stages (i), (ii), and (iii).



Vortex loops in $RMnO_3$



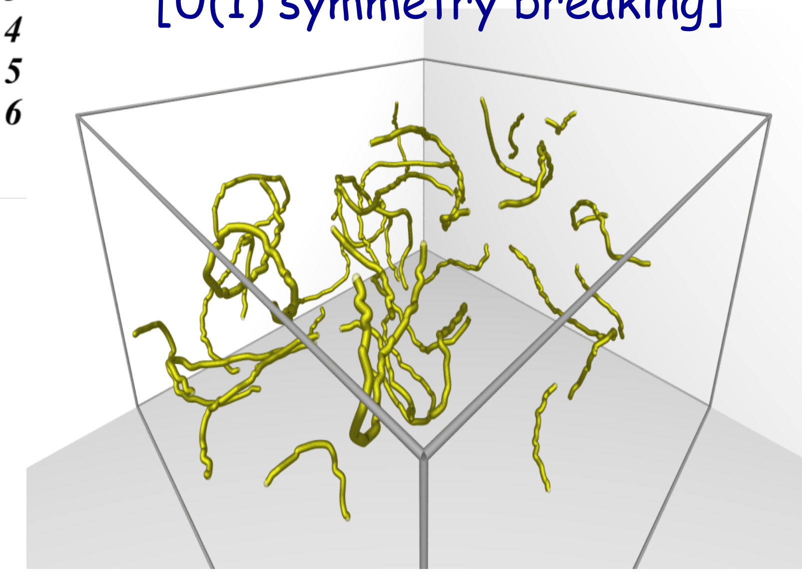
$LuMnO_3$

L. Onsager

R. P. Feynman

Similar idea for the superfluid transition in ^4He
[U(1) symmetry breaking]

Monte Carlo simulation



Theory for vortices

Direct description

Kleinert, "Gauge Fields in Condensed Matter" (World Scientific)

$$\mathcal{H}_\phi = m_\phi^2 \phi^2 + u_\phi \phi^4 + \frac{1}{2} (\nabla \phi)^2$$

⇨ This may be analyzed, e.g., by the ε-expansion

cf. Wilson-Fisher fixed point

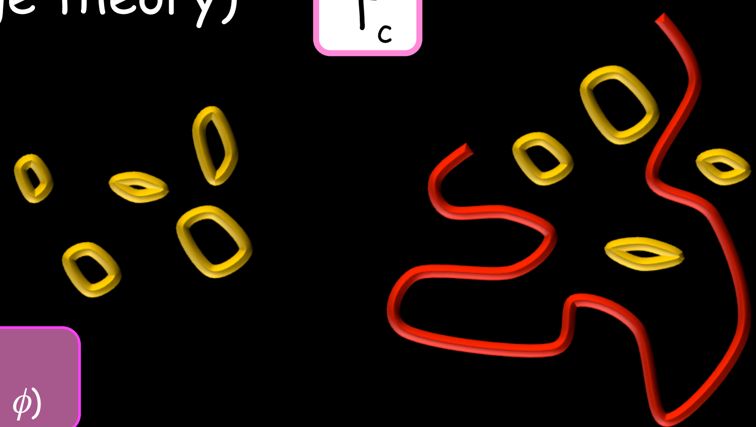
low-T — broken symmetry — U(1) (emergent) — T_c — symmetric phase (Z_6) — high-T

Dual description (gauge theory)

Coulomb phase

Biot-Savart coupling between vortex-line segments

photon (= Goldstone mode of ϕ)



Higgs phase

supercurrent of ψ (= global vortex line of ϕ)

screening

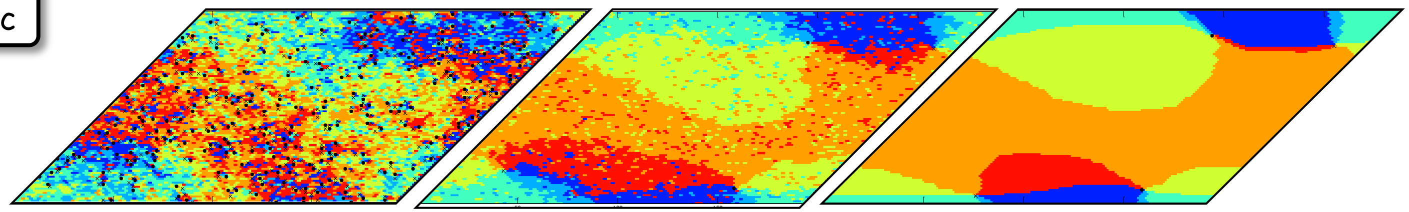
Disorder Field Theory

$$\mathcal{H}_\psi = m_\psi^2 \psi^2 + u_\psi \psi^4 + \frac{1}{2t} \left| \left(\nabla - i q_{\mathrm{eff}} \mathbf{A} \right) \psi \right|^2 + \frac{1}{2} (\nabla \times \mathbf{A})^2$$

Initial condition of cooling : $T_{init} > T_c$ or $T_{init} < T_c$

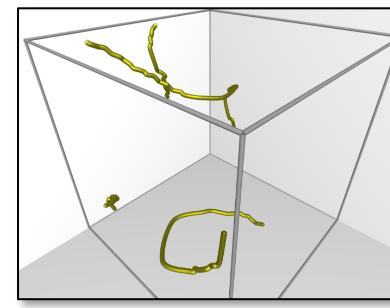
—simulation—

Cooling from $T > T_c$

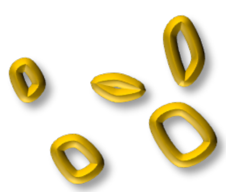


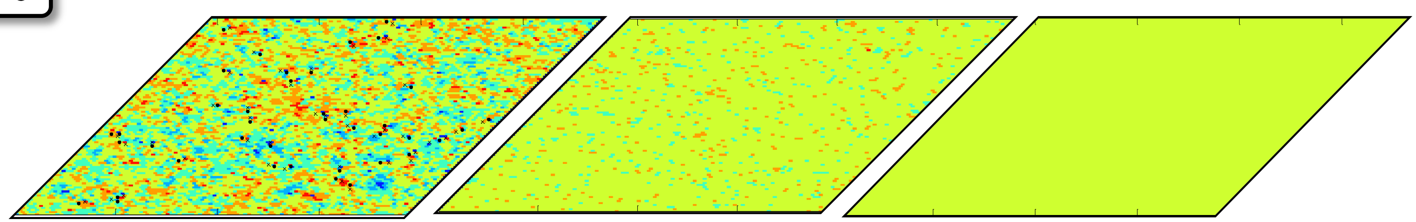
annealing

If cooled down from $T > Tc$, percolating vortex lines remain in the final state.



Cooling from $T < T_c$



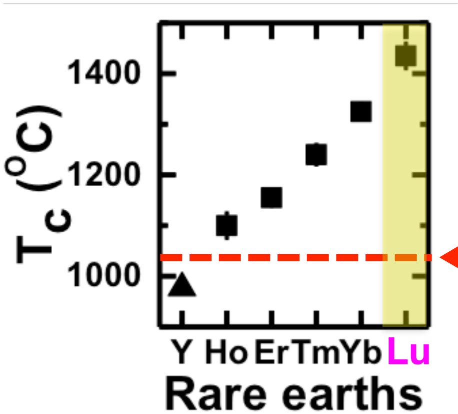


annealing

No vortex line left in the final state

Initial condition of cooling : $T_{init} > T_c$ or $T_{init} < T_c$

FE transition T

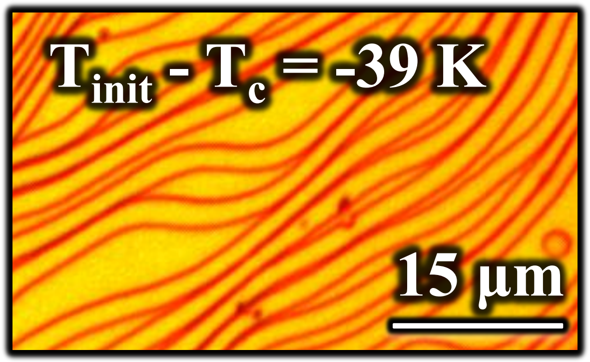


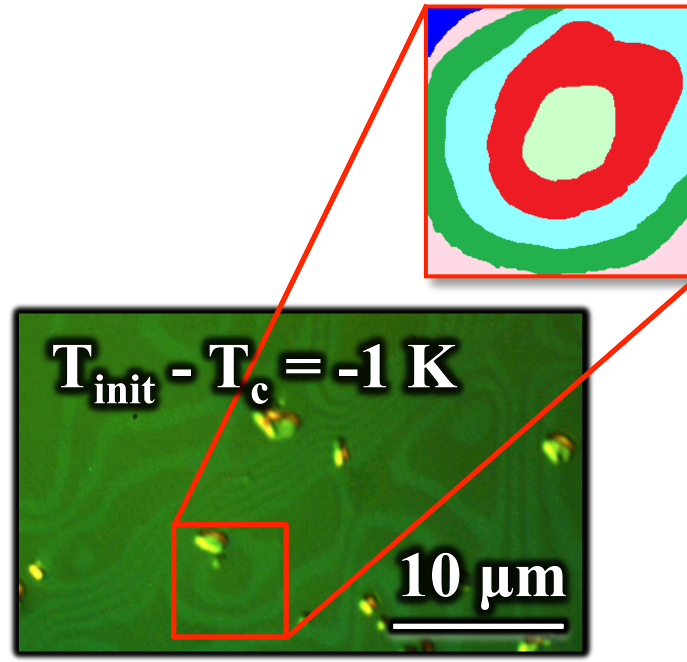
—experiments—

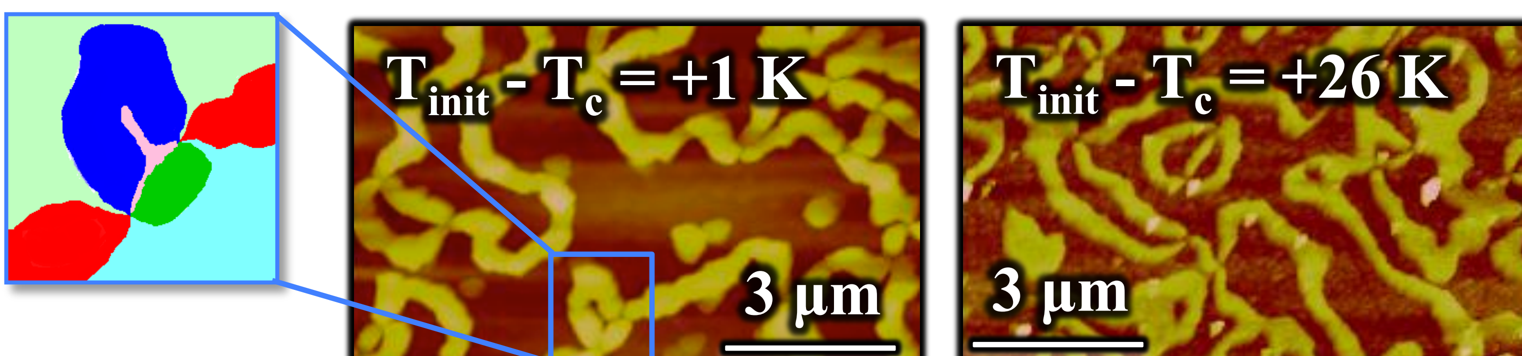
$LuMnO_3$ (T_c = 1672 K)

Crystal growth @T < T_c

Crystal growth temperature



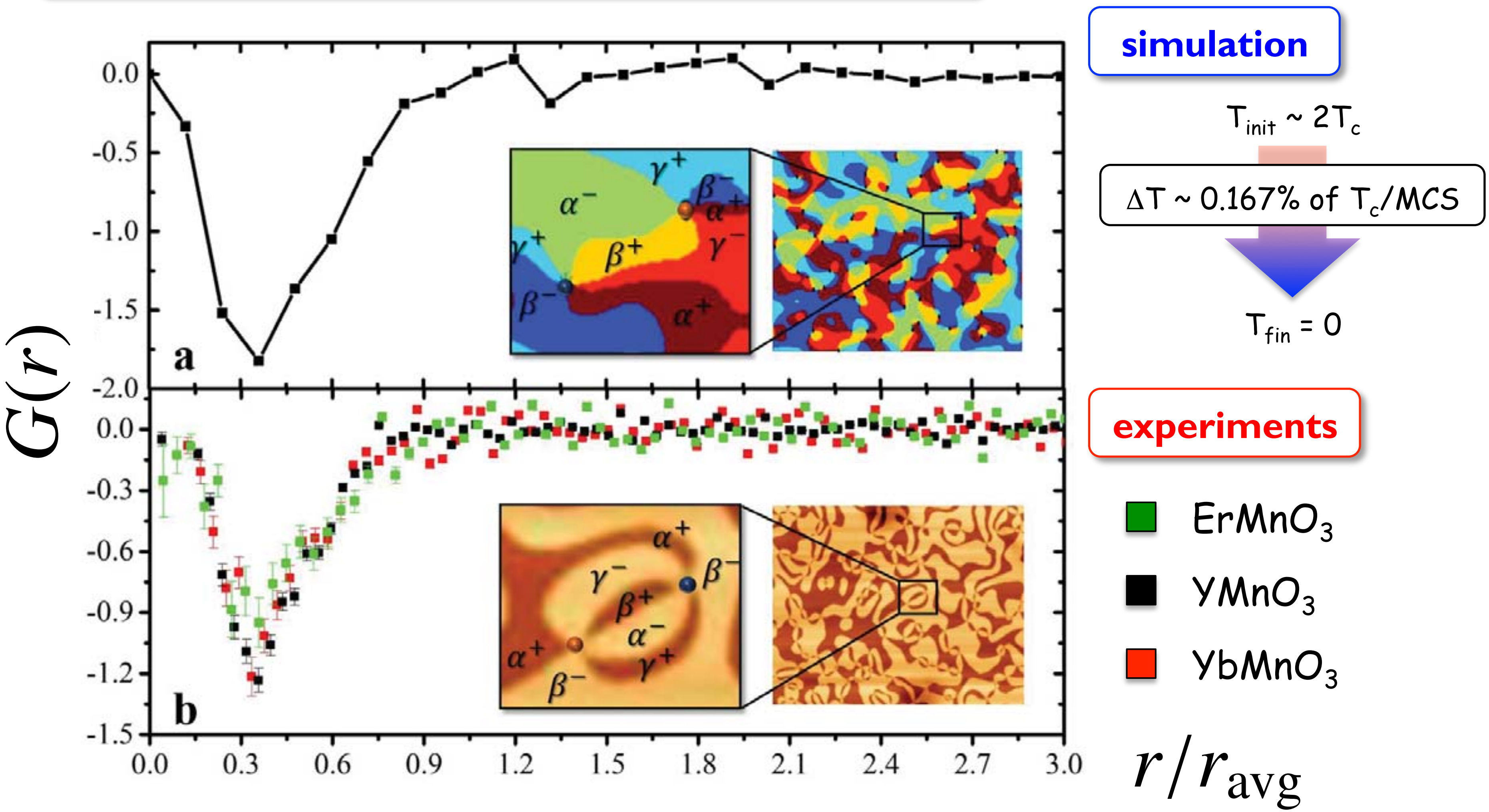




Frozen vortex-antivortex pairs

$$G(r) = \langle \rho(0)\rho(r) \rangle\,, \quad \rho(r) = \sum_{\alpha:\ \text{vortex index}} q_\alpha \delta(r - r_\alpha)$$

q = +1 (-1) for a (anti-)vortex



Kibble-Zurek mechanism

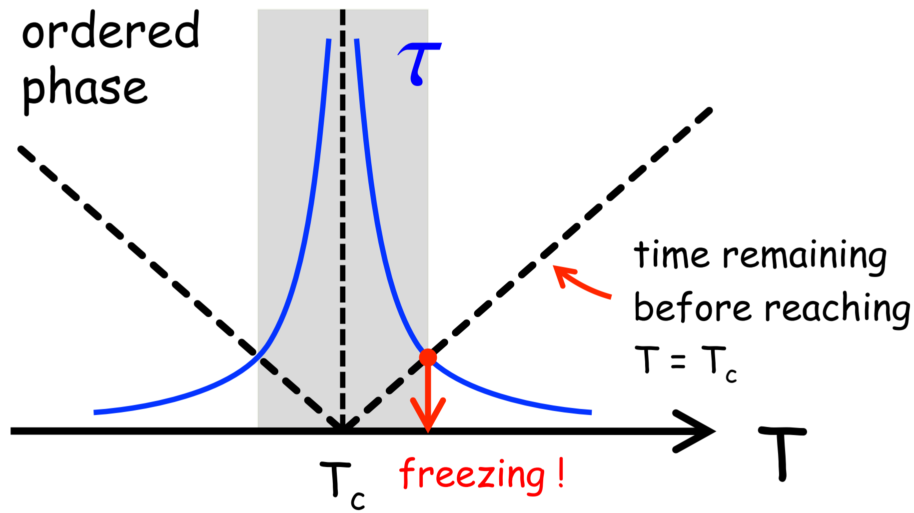
http://en.wikipedia.org/wiki/Kibble-Zurek_mechanism
(and ref's therein)

Suppose T is lowered linearly with time (starting from t < 0) :

$$\varepsilon \equiv (T - T_c)/T_c = -\frac{t}{t_Q}$$

At 2nd order transitions, "critical slowing down" occurs with an exponent z × ν :

$$\tau \sim \xi^z \sim \varepsilon^{-z\nu}$$



When the relaxation time exceeds the time left to reach T_c, the dynamics becomes non-adiabatic.

Freezing condition

$$\tau = \frac{-\varepsilon}{\partial\varepsilon/\partial t} \; (= t_Q \varepsilon)$$

$$\varepsilon_f \sim t_Q^{-1/(1+z\nu)}$$

Size of frozen structures

$$\xi_f \sim t_Q^{\nu/(1+z\nu)}$$

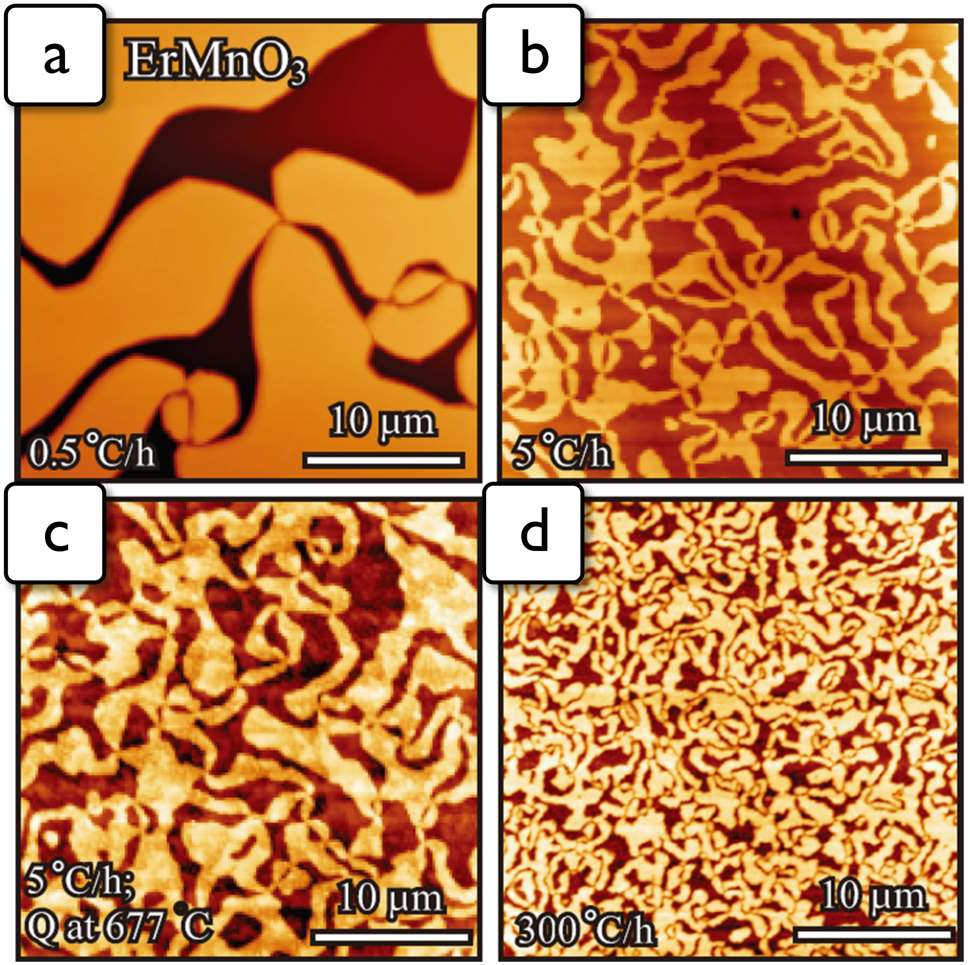
Cross-section density of frozen vortices

$$n_{\mathrm{v}}^{\mathrm{KZM}} \sim \frac{1}{\xi_{\mathrm{f}}^{2}} \sim t_{\mathrm{Q}}^{-\frac{2\nu}{1+z\nu}}$$

$z \sim 2$, $\nu \sim 0.67155(27)$

Campostrini et al., PRB 2001

$$\Rightarrow \frac{2\nu}{1+z\nu} \approx 0.57$$



$ErMnO_3$ (T_c = 1403 K)

Fig	initial T	cooling rate
(a)	1493 K (+90 K)	0.5 K / h
(b)	1473 K (+70 K)	5 K / h
(c)	1473 K (+70 K)	5 K / h quench to RT @ 950 K
(d)	1473 K (+70 K)	300 K / h

Chae et al., PRL 2012

Cross-section density of frozen vortices

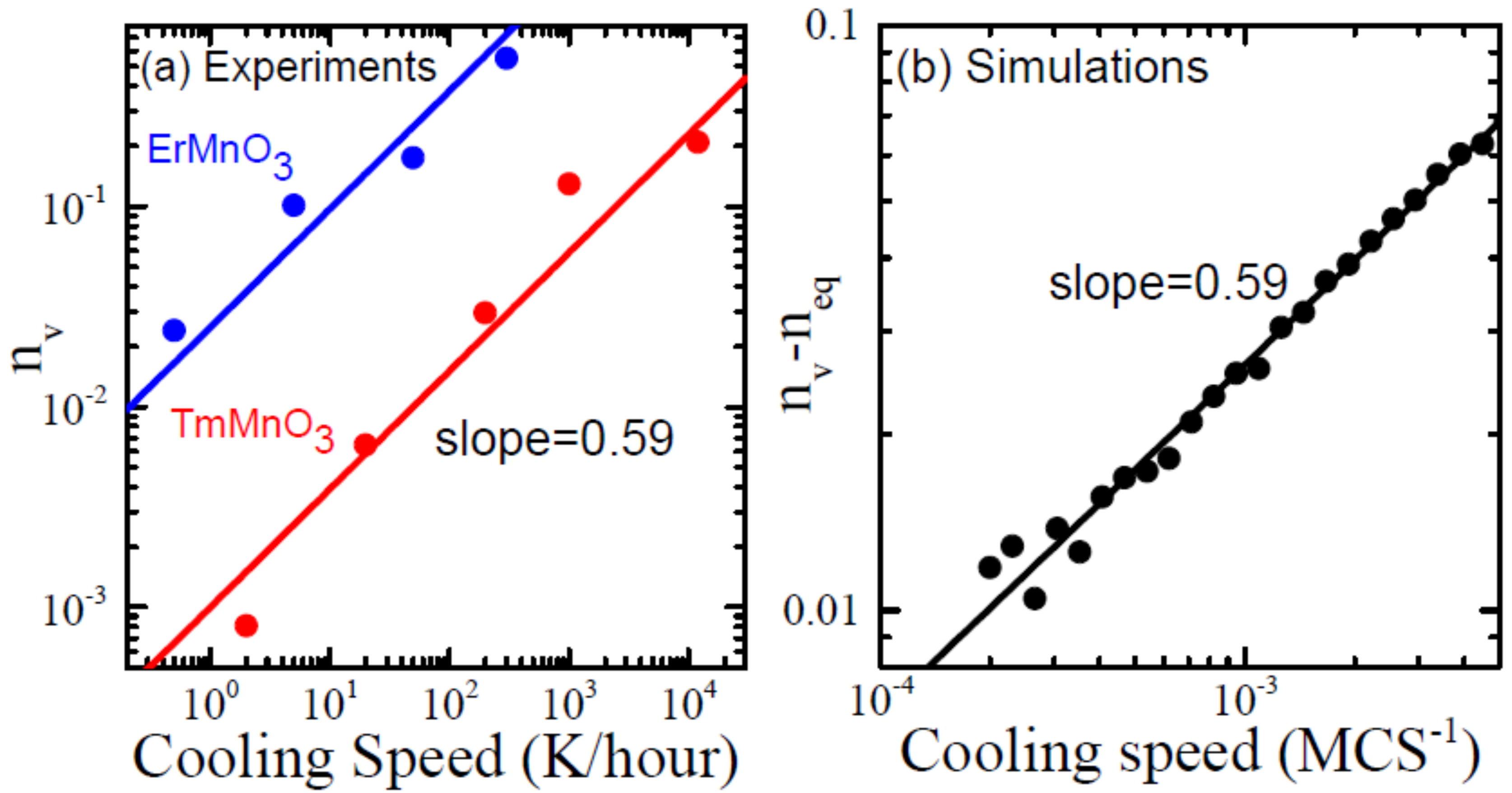
$$n_{\mathrm{v}}^{\mathrm{KZM}} \sim \frac{1}{\xi_{\mathrm{f}}^2} \sim t_{\mathrm{Q}}^{-\frac{2\nu}{1+z\nu}}$$

z ~ 2, ν ~ 0.67155(27)

Campostrini et al., PRB 2001

$$\Rightarrow \frac{2\nu}{1+z\nu} \approx 0.57$$

experiments **simulation**



Summary

- Direct observation of the 3D XY transition driven by proliferation of vortex loops in hexagonal $RMnO_3$
- The 6-state clock model serves as a good effective model
- The sharp asymmetry between cooling from $T > T_c$ or $T < T_c$ is a consequence of the Higgs condensation of vortex lines
- The Kibble-Zurek mechanism to explain the frozen vortex density after a rapid cooling is confirmed both in experiments and numerical simulations