Connectivity of topological defects in nematic liquid crystals confined in complex geometries

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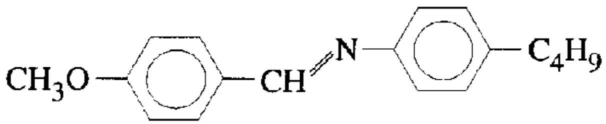
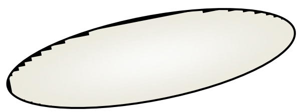
Special Thanks to Akira Onuki (Kyoto Univ.)

GCOE Symposium Links among Hierarchies
at Kyoto, February 14, 2012

Liquid crystal

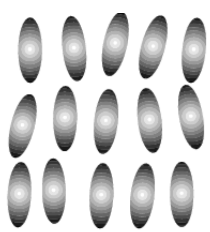


n-4'-MethoxyBenzylidene-n-ButylAnilin (MBBA)



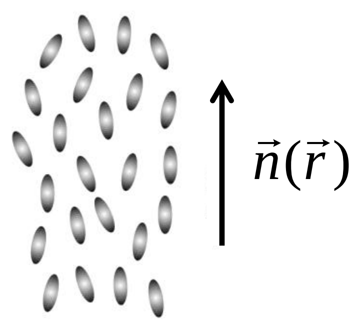
Liquid crystals are intermediate phases between liquid and crystal.
Typically, they are consisted of rod-like molecules.

smectic



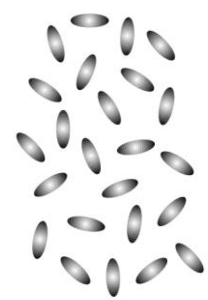
orientational order and layering

nematic

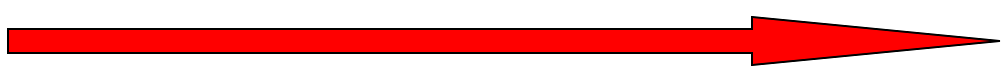


orientational order

isotropic

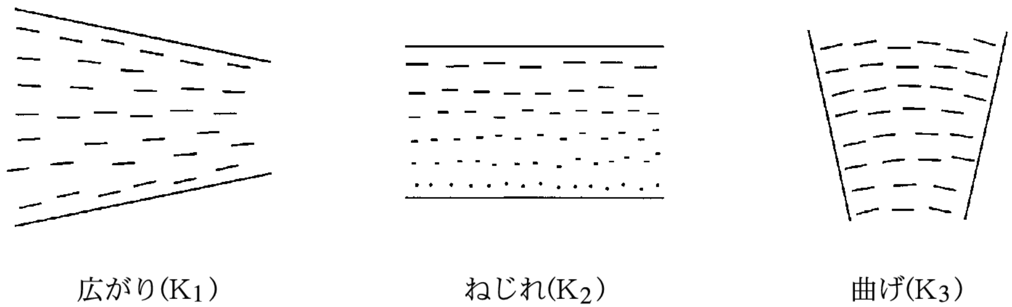


disorder (Liquid phase)



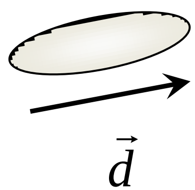
temperature

Elasticity of nematic phase



spray (K_1) twist (K_2) bend (K_3)

$$Q\left(n_\alpha n_\alpha - \frac{1}{3}\delta_{\alpha\beta}\right) = \left\langle d_\alpha d_\alpha - \frac{1}{3}\delta_{\alpha\beta}\right\rangle_{\mathrm{local}}$$



local director field $\vec{n}$ $(|\vec{n}|=1)$

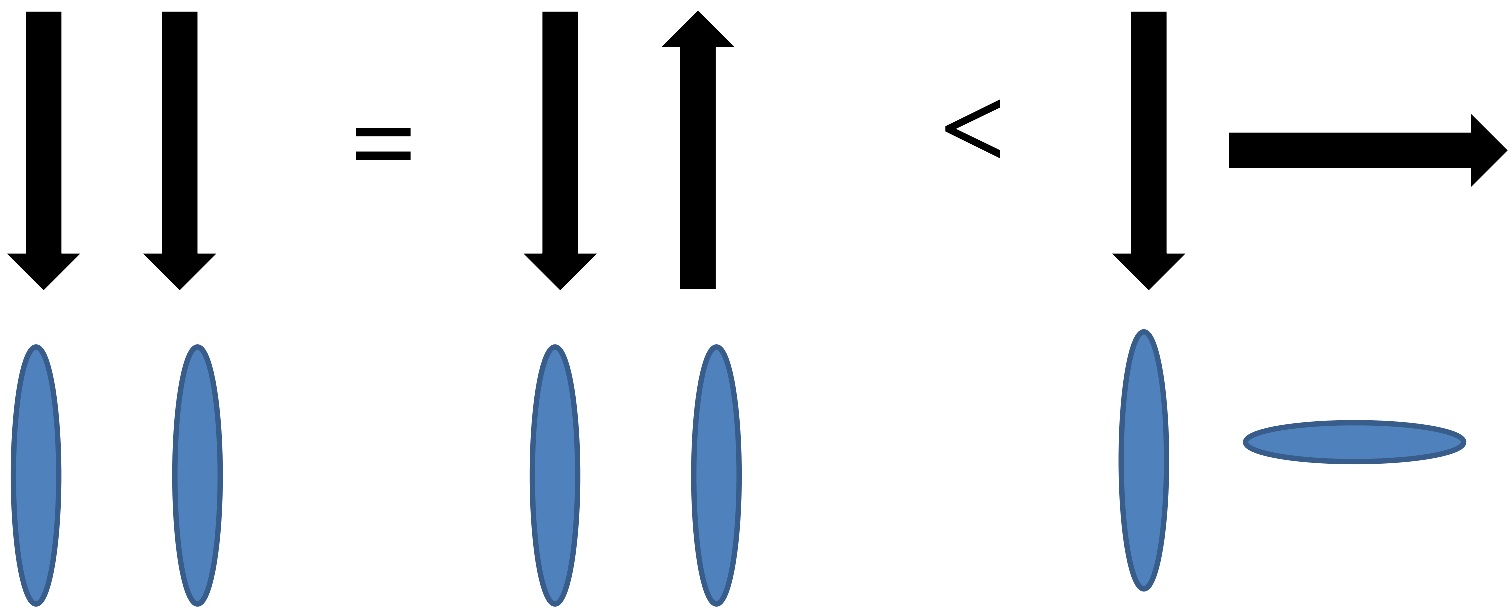
scalar nematic order Q

Frank elastic energy
$$F = \int d\vec{r}\left[\frac{1}{2}\{K_1(\vec{\nabla}\cdot\hat{n})^2 + K_2(\hat{n}\cdot(\vec{\nabla}\times\hat{n}))^2 + K_3(\hat{n}\times(\vec{\nabla}\times\hat{n}))^2\right]$$

Lebwohl-Lasher
$$H = -J\sum_{\langle i,j\rangle}(\vec{n}_i\cdot\vec{n}_j)^2$$

Symmetry of Liquid crystal

In contrast to Heisenberg spins, there is no difference between head and tail of the director field in nematic phase.



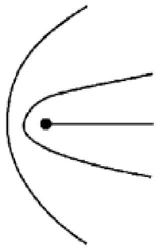
order parameter space

Lebwohl-Lasher $H = -J \sum_{\langle i,j \rangle} (\vec{n}_i \cdot \vec{n}_j)^2$ $S_2 / Z_2 \quad (RP_2)$

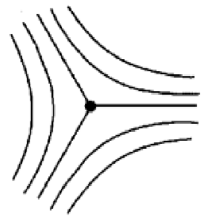
Heisenberg $H = -J \sum_{\langle i,j \rangle} \vec{n}_i \cdot \vec{n}_j$ S_2

Defects in liquid crystals

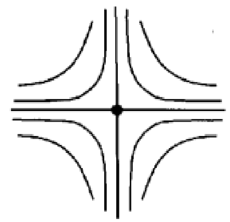
When incommensurate domains contact, topological defects are formed at the domain boundary



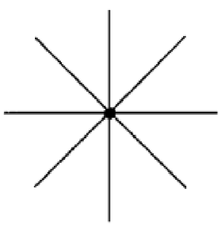
$s = 1/2$



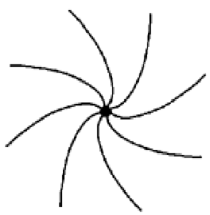
$s = -1/2$



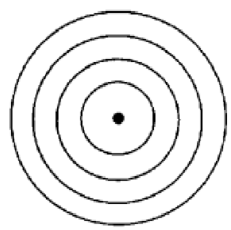
$s = -1$



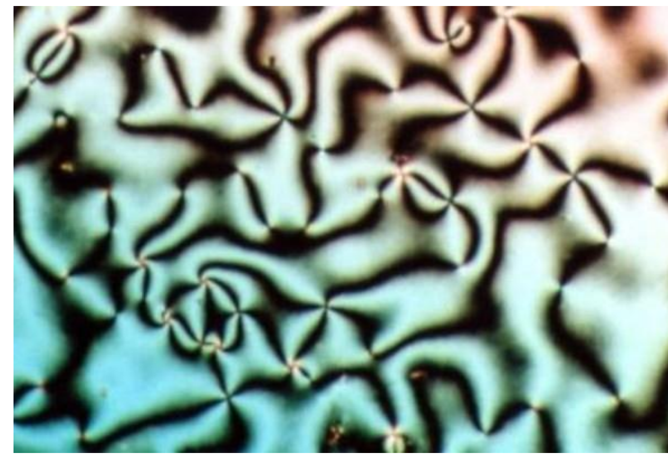
$s = +1, \theta_0 = 0$



$s = +1, \theta_0 = \pi / 4$



$s = +1, \theta_0 = \pi / 2$



Schlieren texture

$$\phi(\vec{r}) = s\theta(\vec{r}) + \theta_0$$

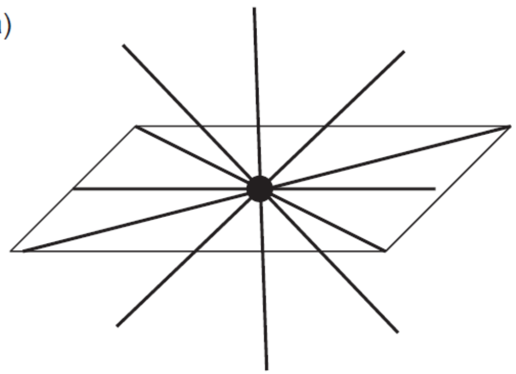
θ : angular coordinate
ϕ: angle of director field
s: the strength of the defect

defect core energy $E_d = \frac{1}{K}\int d\vec{r}\left(\nabla\phi\right)^2 \propto s^2$

Defects of nematic phase in 3D

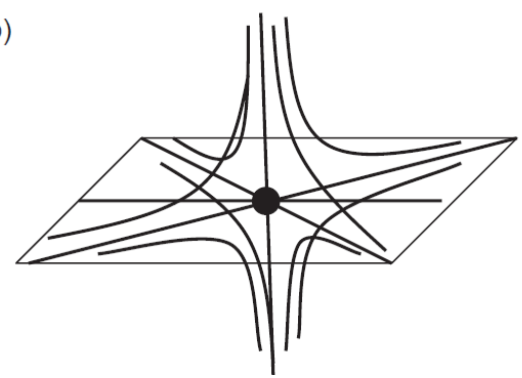
point defects

(a)



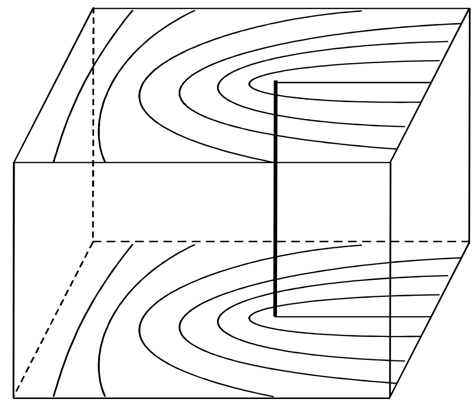
$s = 1$

(b)

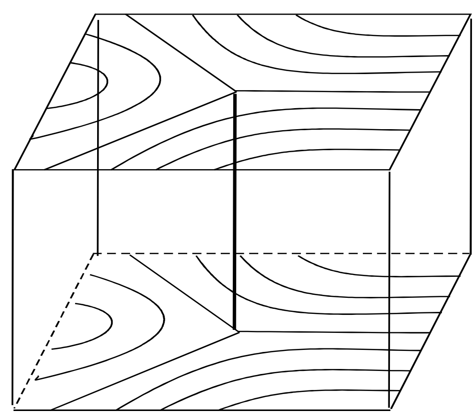


$s = -1$

Line defects
(disclinations)



$s = 1/2$



$s = -1/2$

Homotopy theory

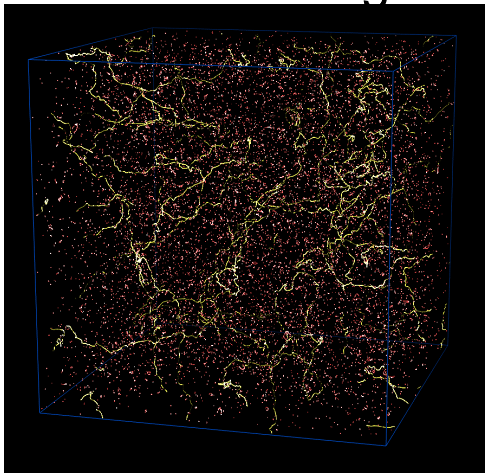
$$\pi_0(S_2 / Z_2) = 0$$

$$\pi_1(S_2 / Z_2) = Z_2$$

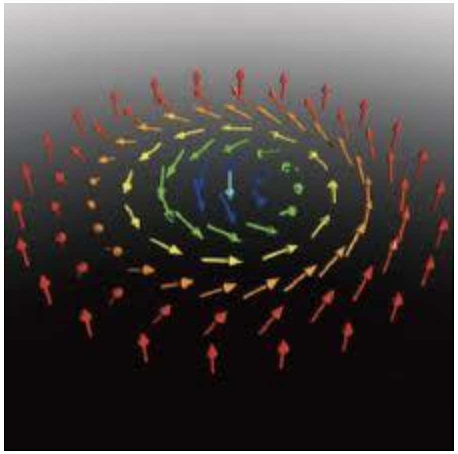
$$\pi_2(S_2 / Z_2) = Z$$

Topological Defects in other systems

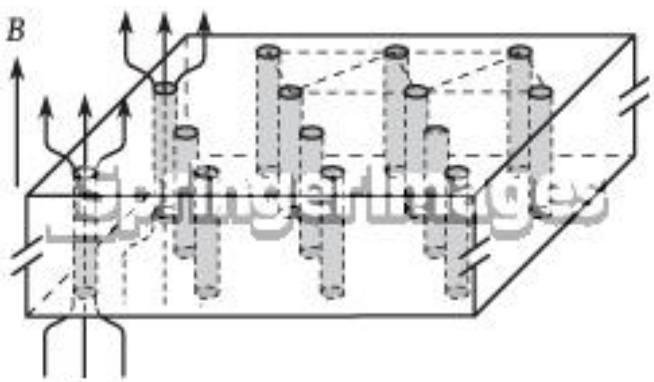
Cosmic strings



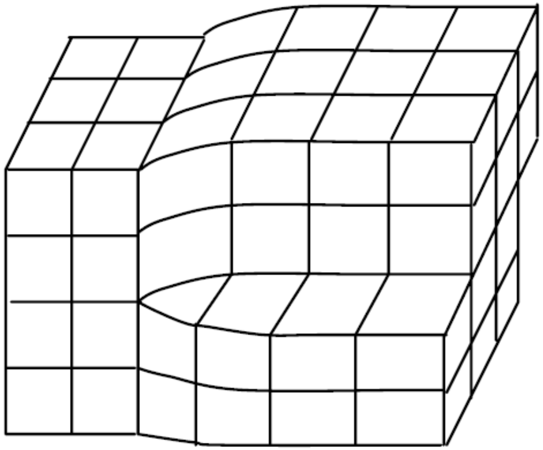
Skyrmion



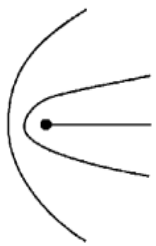
Type II superconductors



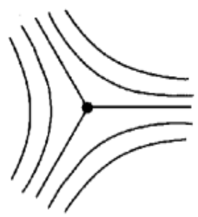
Dislocations in crystals



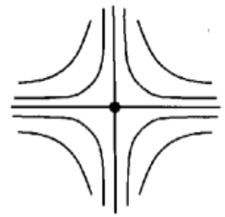
Defects in liquid crystals



$s=+\frac{1}{2}$

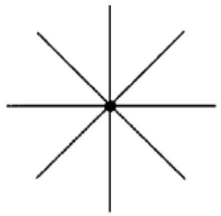


$s=-\frac{1}{2}$



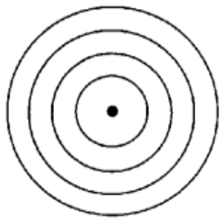
$s=-1$

A defect of s interacts with that of s'.
Roughly, the strength of the interaction is proportional to ss'.



$s=+1, \theta_0=0$

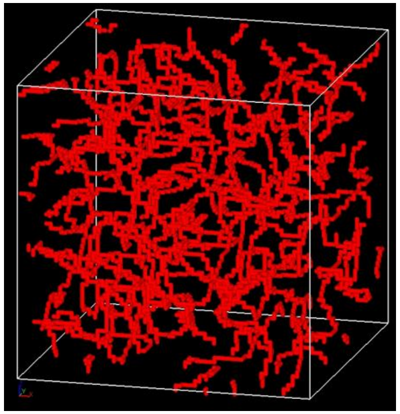
$s=+1, \theta_0=\frac{\pi}{6}$



$s=+1, \theta_0=\frac{\pi}{2}$

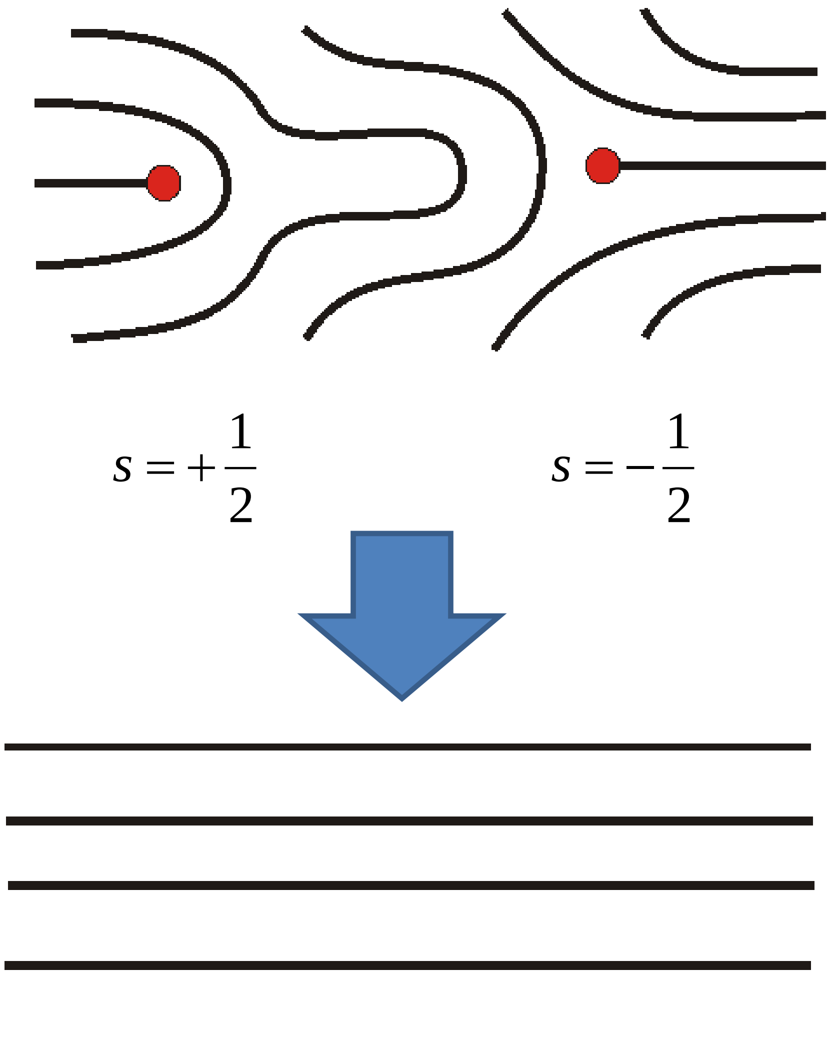
(+,+) and (-,-)	: repulsive
(+,-)	: attractive

Analogous to electrostatic interaction



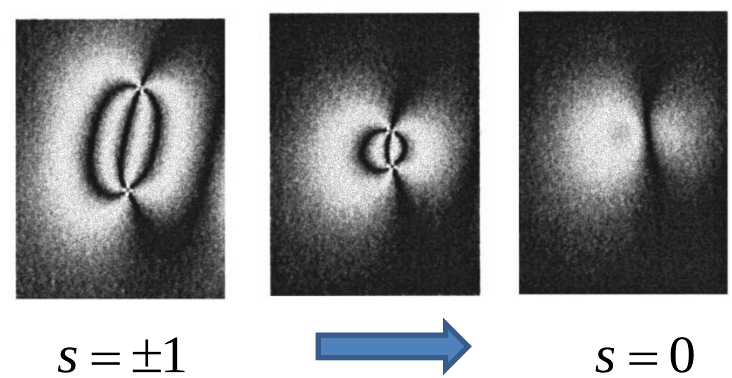
A line defect has a tension in 3D.
It tends to be shrunken.

Annihilation of defects

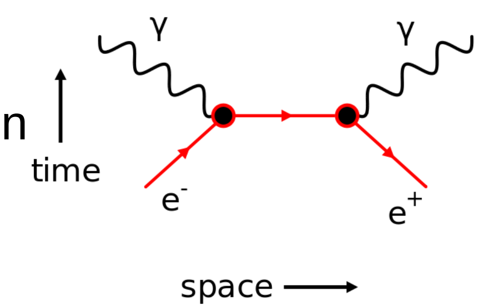


In bulk, defects of nematic phase are not long-lived

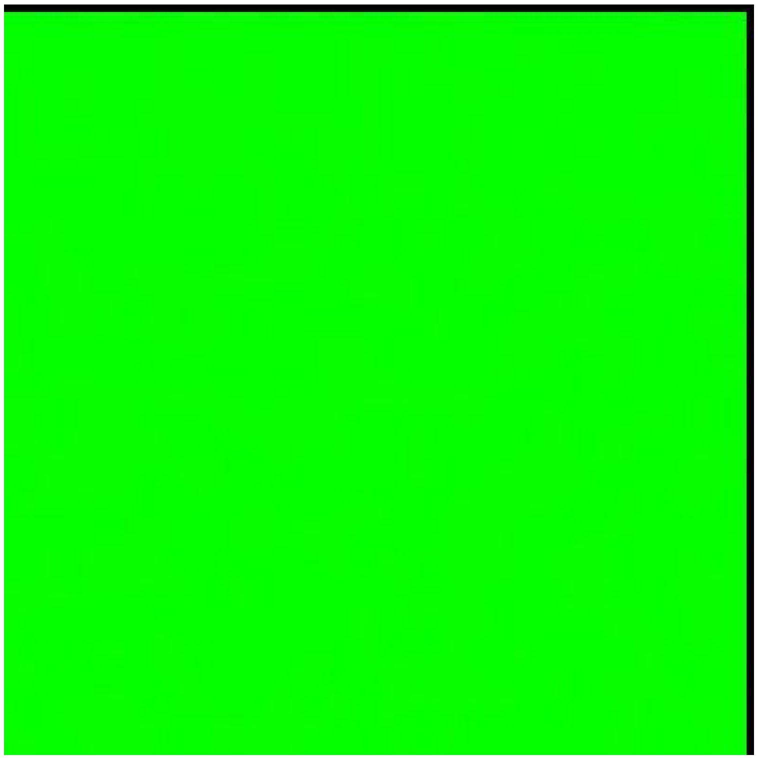
A defect of the topological charge S is annihilated with other one of $-S$

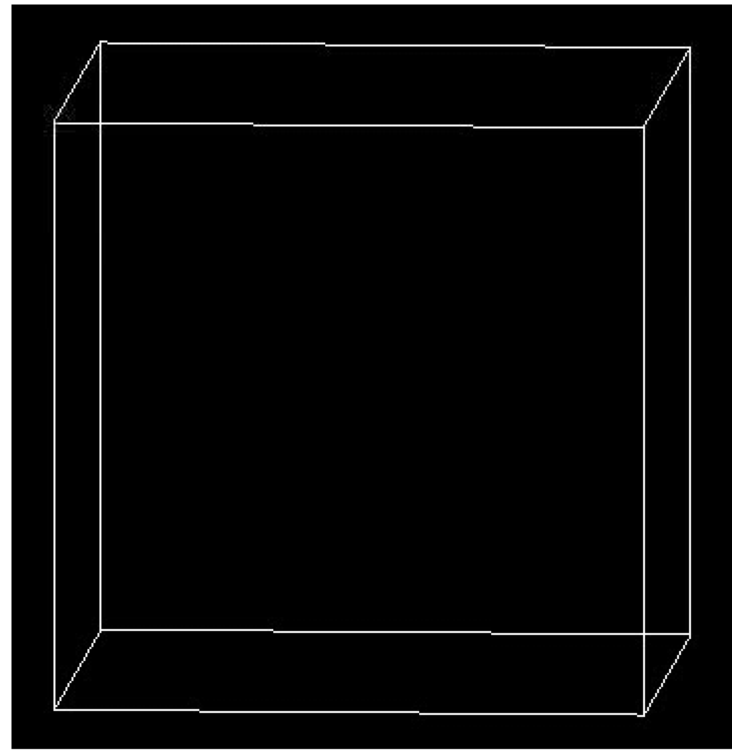


electron-positron annihilation



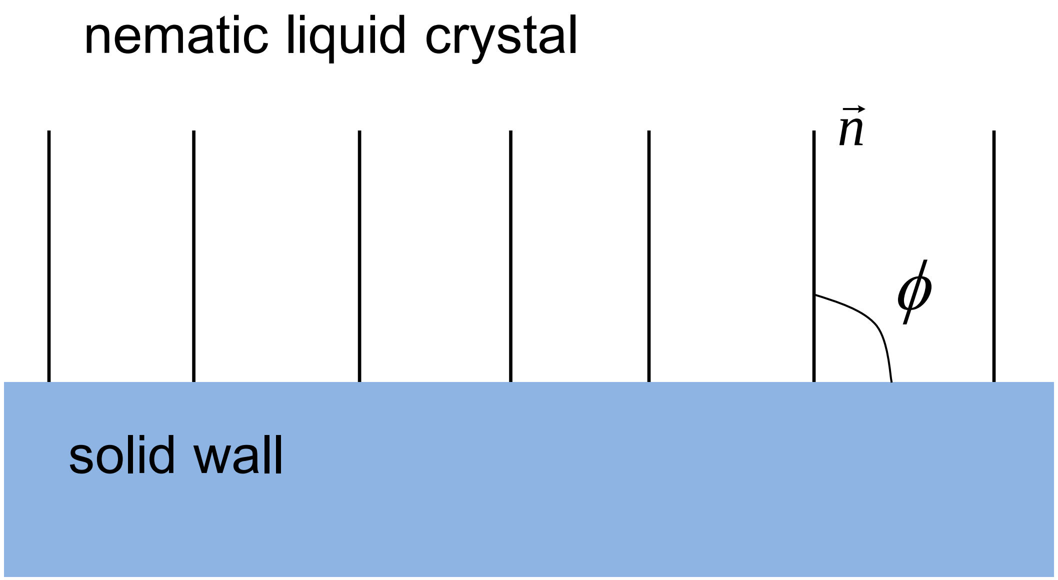
Simulations of nematic ordering





Correlation length
(characteristic separation between defects) $R \propto t^{1/2}$

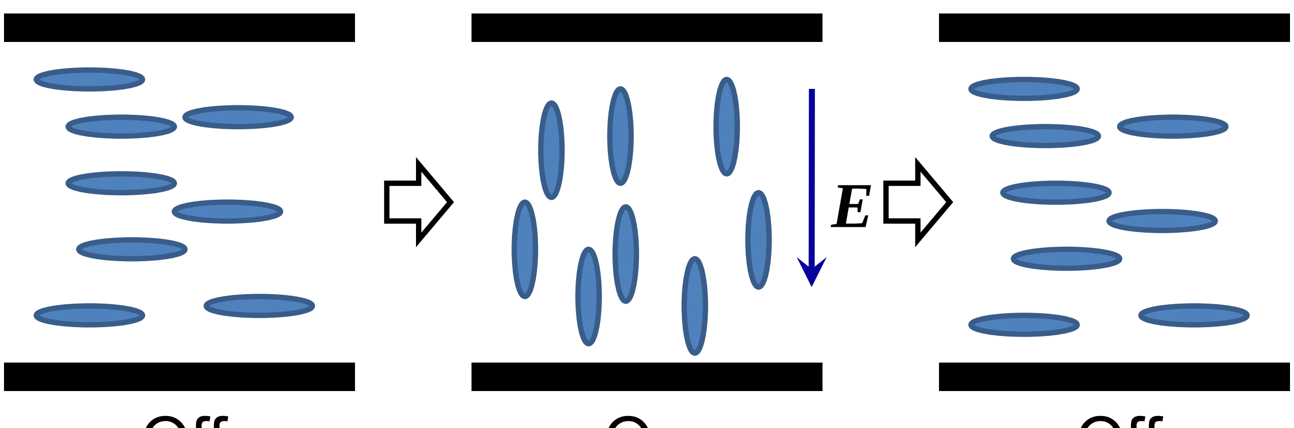
Anchoring interaction



Director field is aligned at solid surface with tilt angle ϕ

$\phi = 90^\circ$ homeotropic

$\phi = 0^\circ$ planar

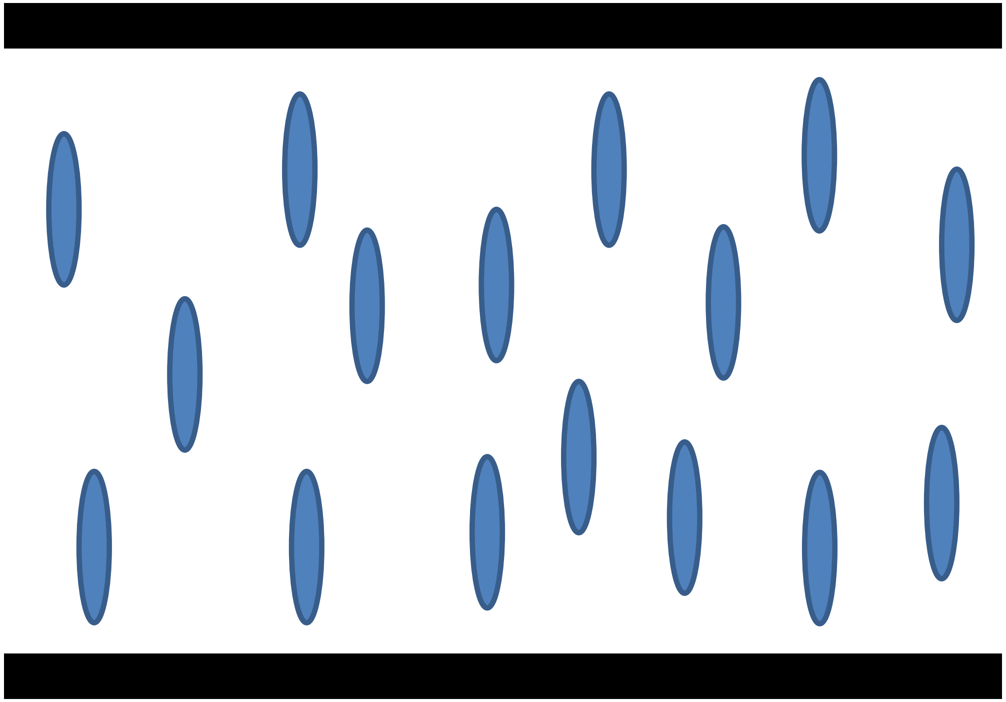


Fredericks transition

$$E_c = \frac{\pi}{d}\sqrt{\frac{K}{\varepsilon_0 \Delta\varepsilon}}$$

Confinement effect

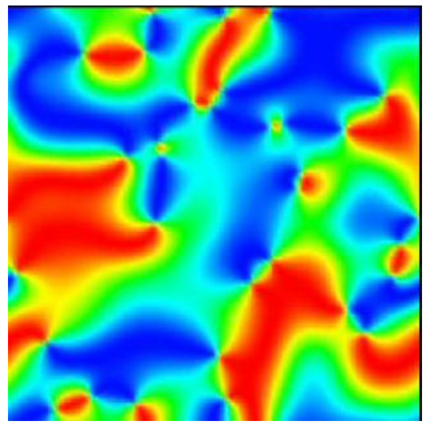
For homeotropic anchoring



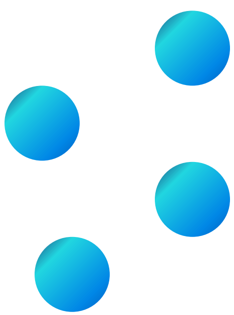
The effect of the anchoring interaction can reach far from the surface owing to the long-ranged elasticity. In between parallel flat walls, the director field can be aligned uniformly.

Liquid crystal and solid objects

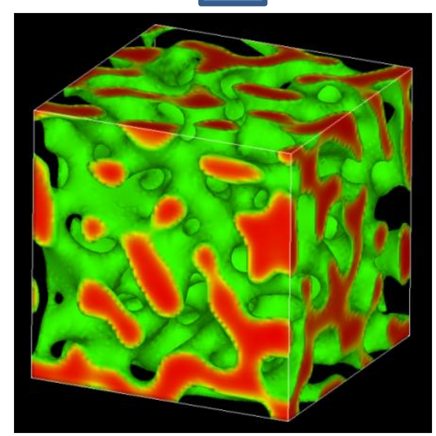
The inclusion of solid objects imposes the formation of defect in liquid crystals



nematic liquid crystal



particles (colloids)

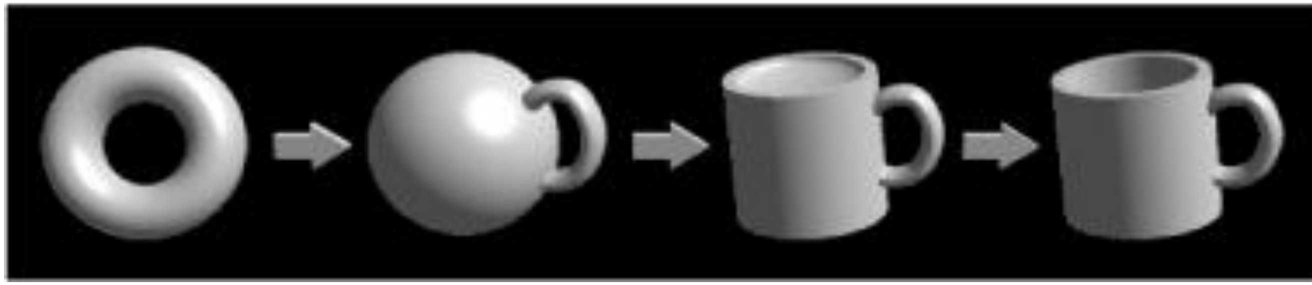


porous media

(Phys. Rev. Lett. 97, 127801 (2006))

(Nature Materials 10, 303 (2011))

Topology of an object



genus $g=0$ $g=1$ $g=2$ $g=3$

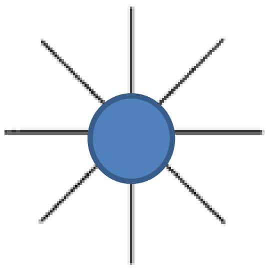
Stein-Gauss theorem $\sum s_i = g-1$ Euler characteristics $\chi = \frac{1}{2\pi}\int dS\overline{\kappa}$

D.L. Stein, Phys. Rev. A 19, 1708 (1979) $= 2-2g$

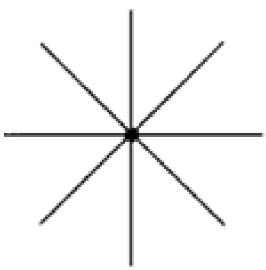
$\sum s_i = 0$ In bulk

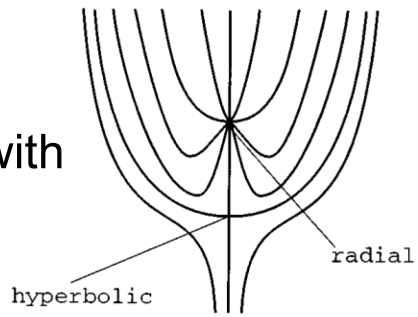
Conservation of the total topological charges

radial

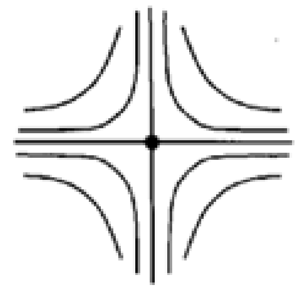


A spherical particle with homeotropic surface

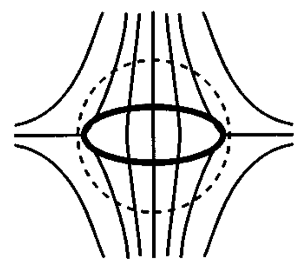




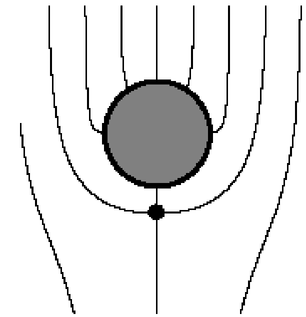
hyperbolic



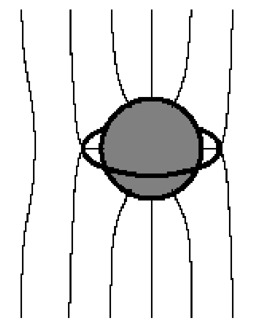
A point defect of $s=-1$



A ring defect of $s=-1/2$



hedgehog (dipole)



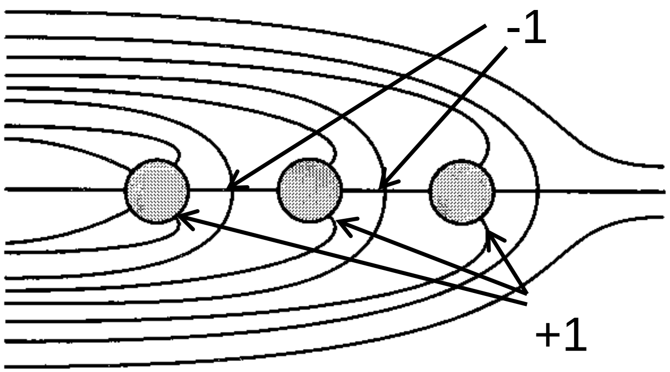
Satrun-ring (quadruple)

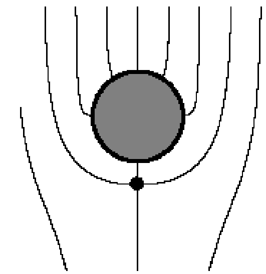
T. C. Lubensky *et al.,* Phys. Rev. E 57, 610 (1998)

The sum of topological charges in the system should be conserved.

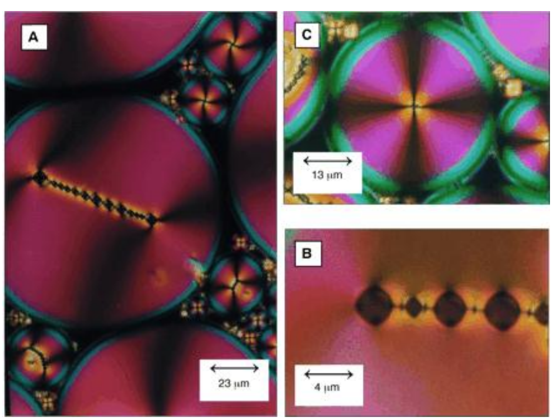
Interaction among particles in LC

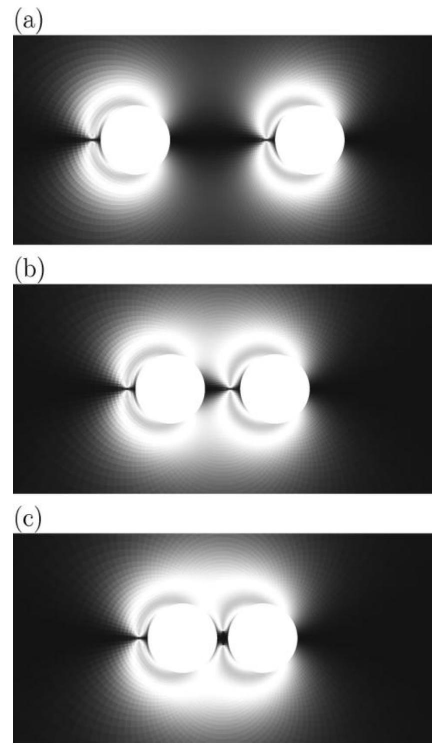
Non-interacting particles can interact to others via a nematic solvent, so as to reduce the elastic energy.

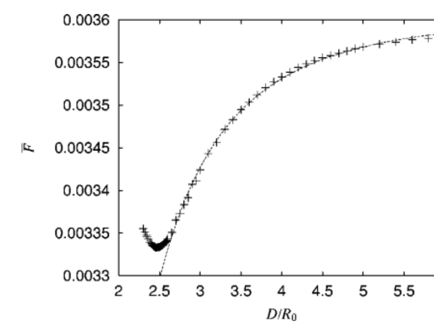




hedgehog
(dipole)





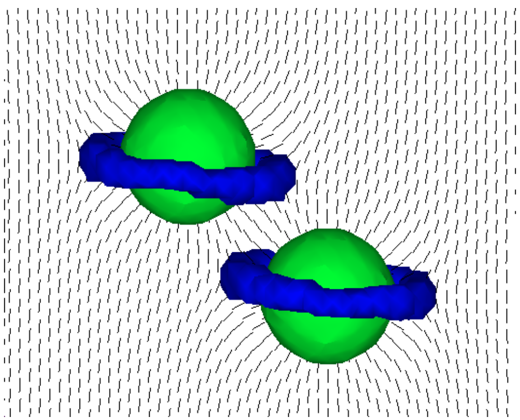


P. Poulin *et al*. Science 275, 1770 (1997).

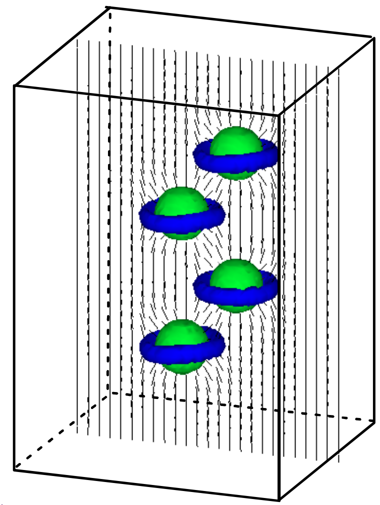
J. Fukuda *et al*. Euro. Phys. J. E. 13. 87 (2004)

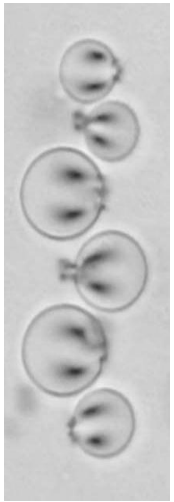
Interaction among particles in nematic solvents

(a)



(b)





K. Kita *et al.*,
Phys. Rev. E 77, 041702 (2008)

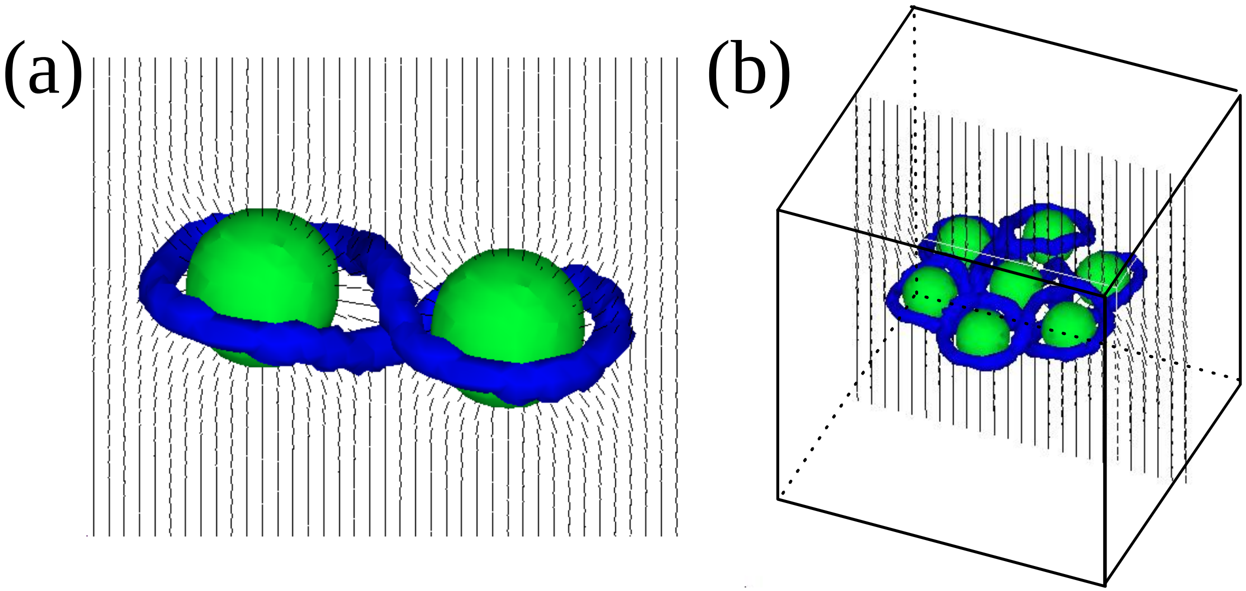
Zig-zag chain-like aggregate

A particle with a Saturn-ring defect has a quadruple symmetry.
Thus, particles are interacting in a quadruple manner.

$$V(r,\theta)=\frac{1}{r^5}(9-90\cos^2\theta+105\cos^4\theta)$$

R. W. Ruhwandl and E. M. Terentjev, Phys. Rev. E 55, 2958 (1997)

Interaction among particles in nematic solvents



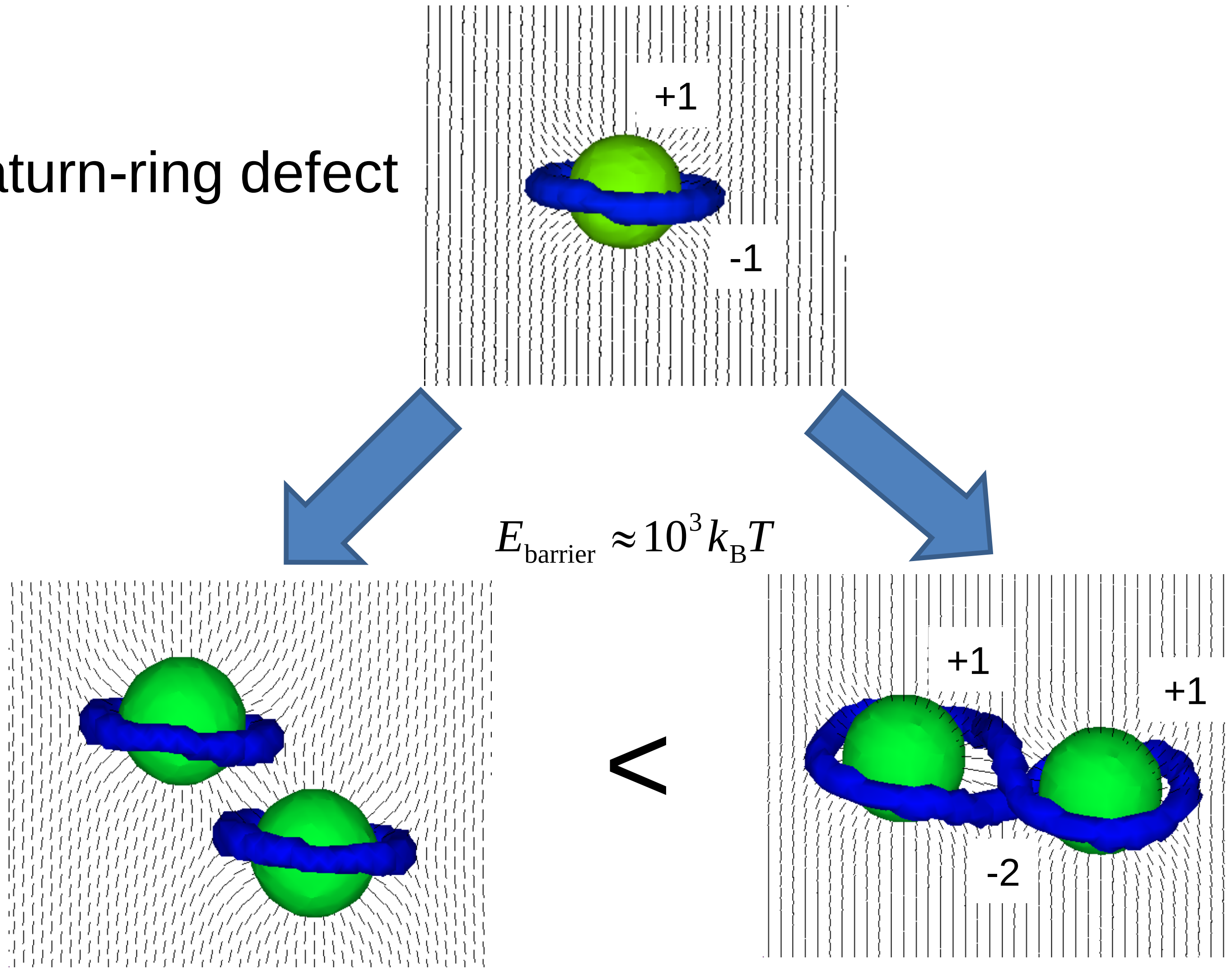
We found a new type of defect around a pair of particles.
It cannot be described by an argument based on the quadruple symmetry.
Defect shared by two particle has figure-of-eight structure and binds particles strongly.

Topological arrest of particles by a single stroke disclination line

T. Araki and H. Tanaka, Phys. Rev. Lett. 97, 127801 (2006)

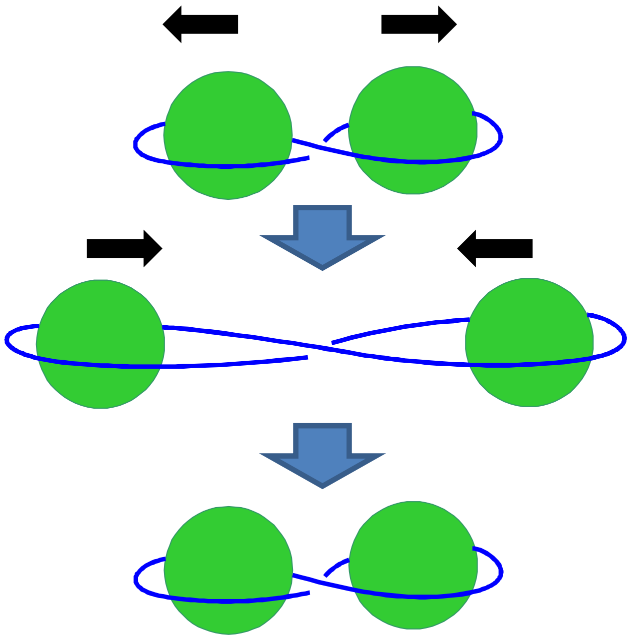
Topology of defect structure

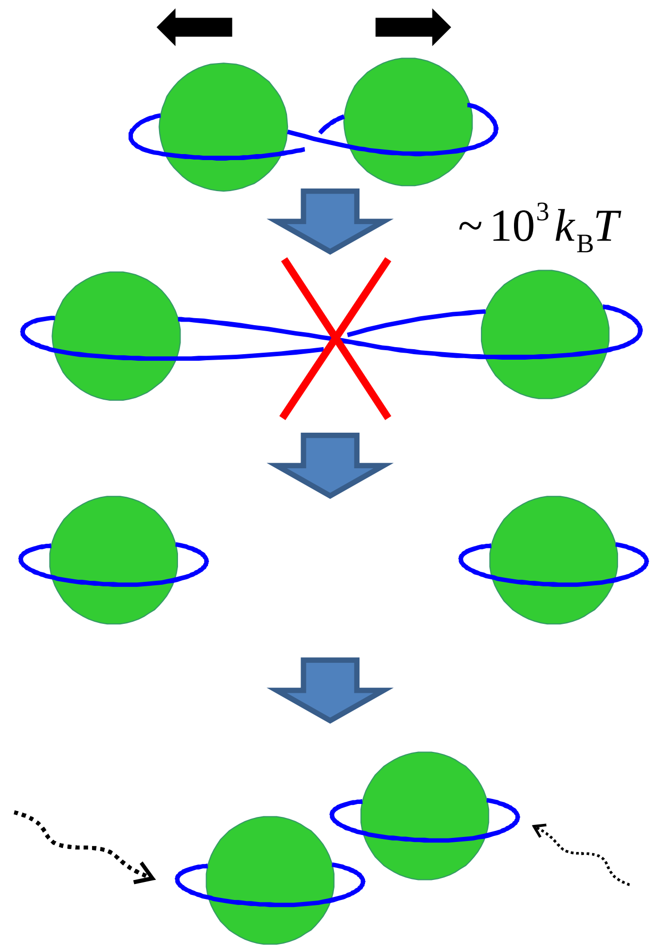
A Saturn-ring defect



Topologically arrested structure

Interaction mediated by defects

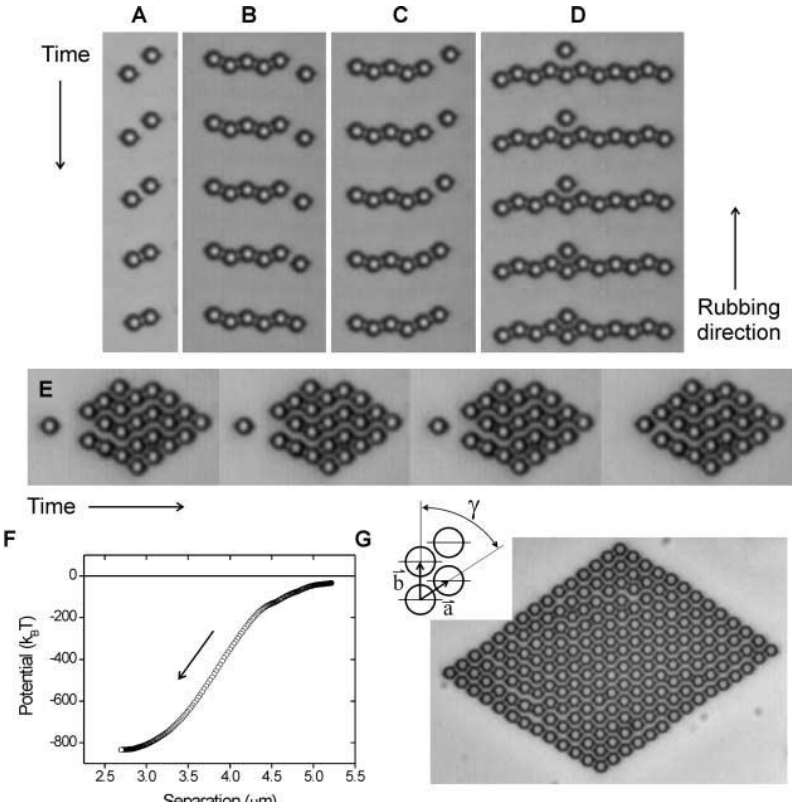




The effective interaction depends on the topology of the defects, so that it is not described by a potential

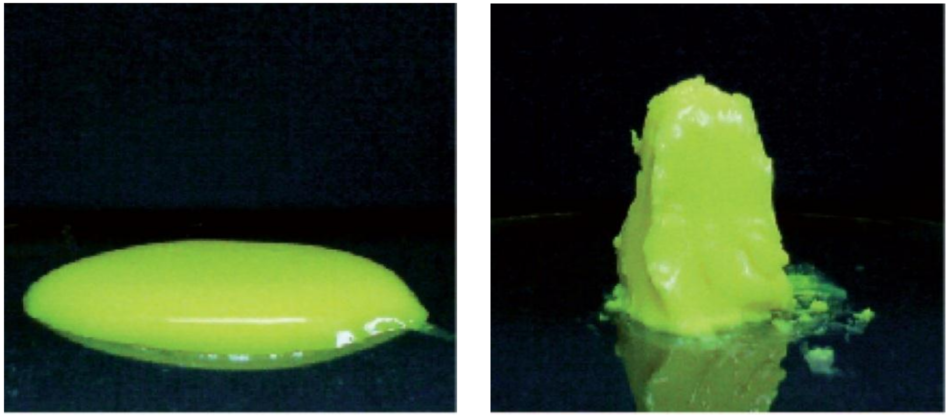
non-additive, non-linear, non-ergodic

Self-assembly by topological defects

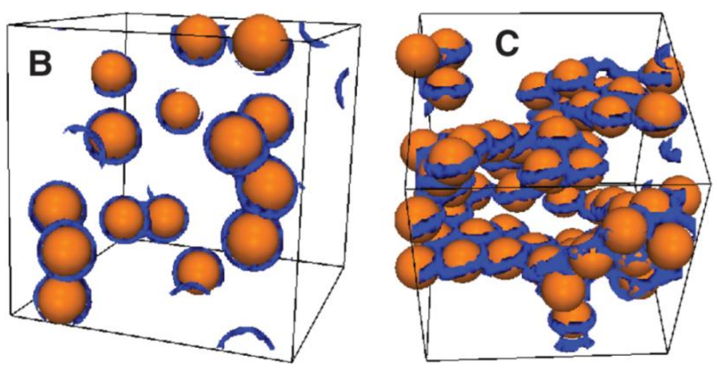


I. Musevic et al. Science 313, 5789 (2006)

5CB+ PMMA beads (49%)

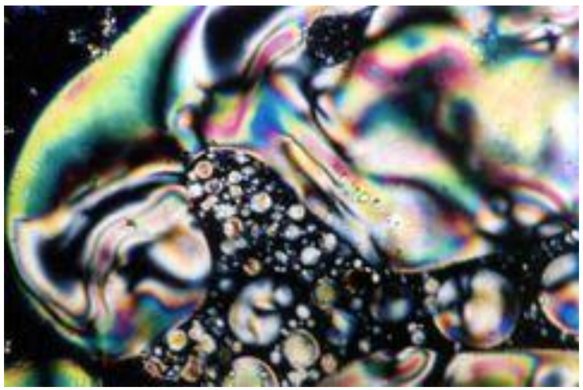


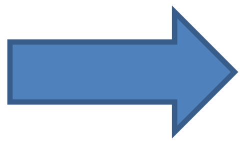
$T > T_c$ $T < T_c$

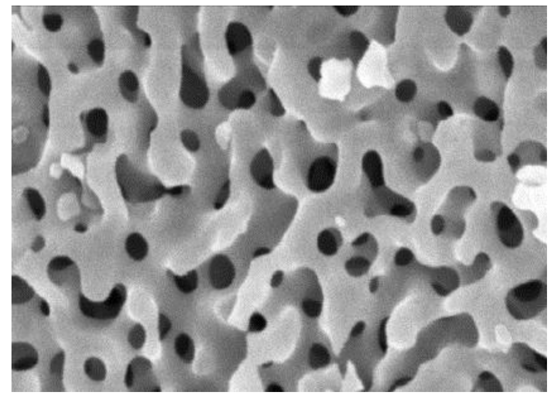


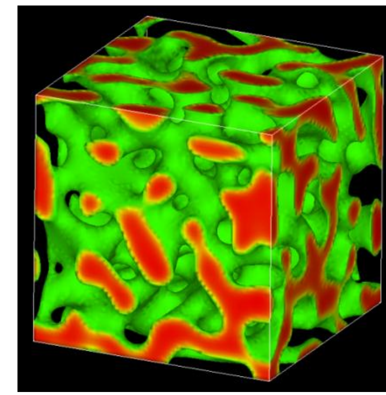
T. A. Wood et al, Science 334, 79 (2011)

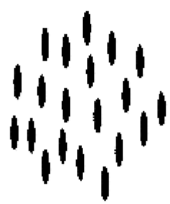
Nematic liquid crystal in porous media











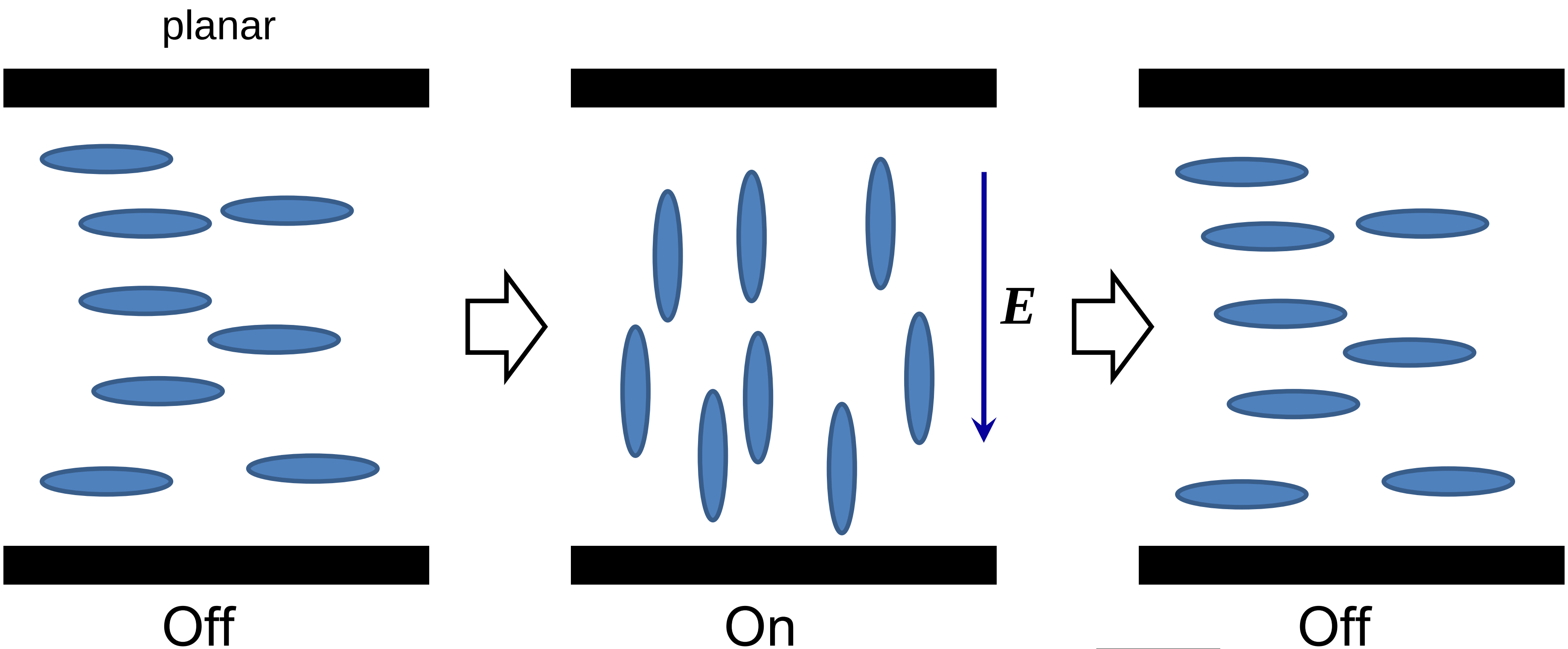
Nematic liquid crystal

porous media(PM)

They show interesting behaviors due to the topological constraints of the defects. And they provide promising properties for optical devices.

G. P. Crawford and S. Zumer, *Liquid Crystals in Complex Geomerty* (1996),
X. Wu et al., Phys. Rev. Lett. 69, 470 (1992).
T. Bellini, Phys. Rev. Lett. 88, 245506 (2002).

Nematic liquid crystal in a simple cell

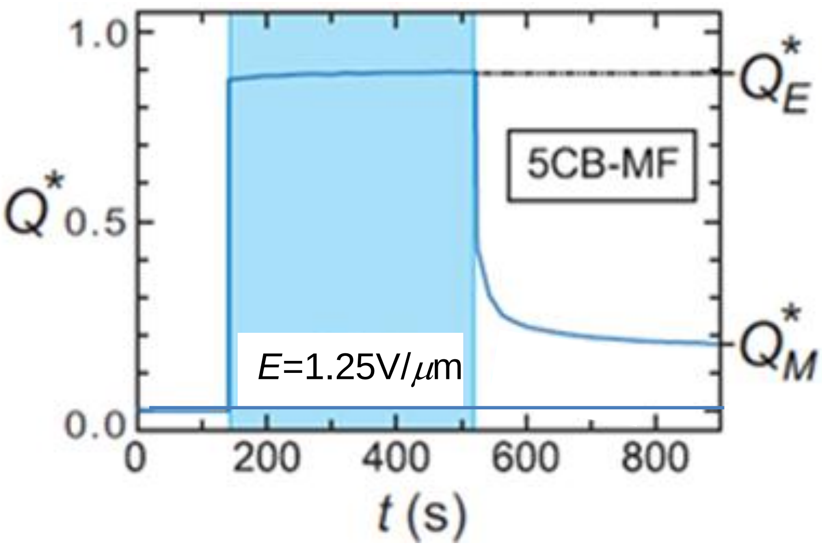


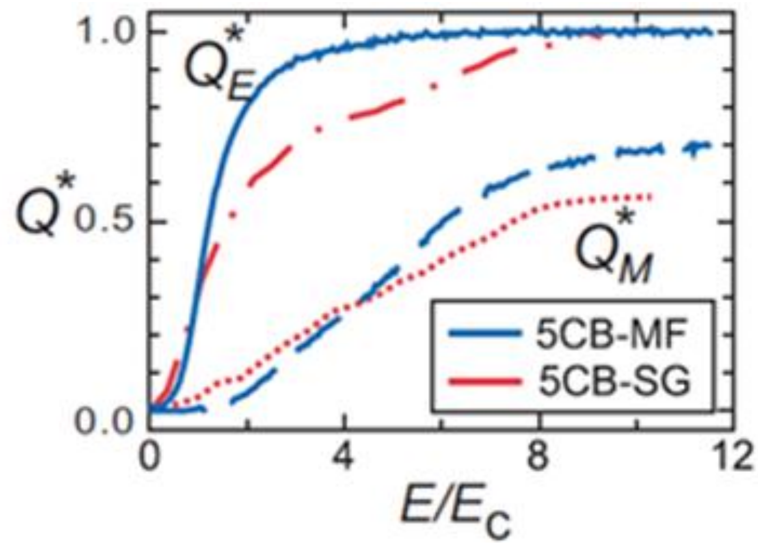
$$E_c = \frac{\pi}{d}\sqrt{\frac{K}{\varepsilon_0 \Delta\varepsilon}}$$

Only a unique direction is recorded in a simple cell.

Memory effects

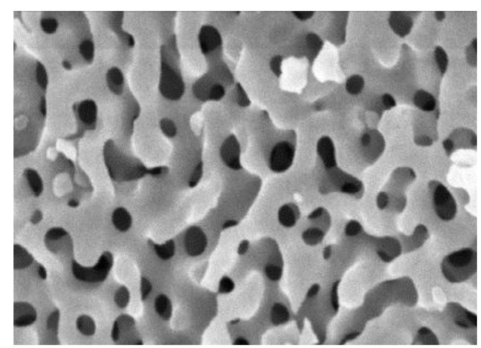
experiments (5CB in millipore filter (3μm) and silica gel (0.8μm))





$$Q^* = \frac{3}{2V}\int d\vec{r}\left(n_z n_z - \frac{1}{3}\right)$$

z // external field



T. Araki *et al.*,Nature Materials 10, 303 (2011)

Nematic liquid crystal in porous media

Since energy barriers between them are higher than the thermal energy, each configuration is trapped at one of the minima.
The systems show non-ergodic glassy behaviors
(analogous to spin-glass)

The effect of the porous media is studied by introducing randomness of the interaction or
point –like quenched impurities

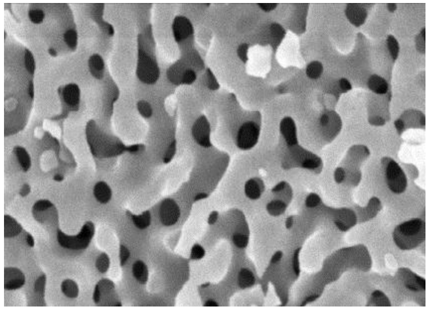
Theory:	A. Maritan *et al*. Phys. Rev. Lett. 72, 4113 (1994),
	L. Petridis and E. M. Terentjev, Phys. Rev. E 74, 051707 (2006).
Simulation:	T. Bellini *et al*. Phys. Rev. Lett. 88, 245506 (2002).
	T. Bellini et al., Phys. Rev. Lett. 85, 1008 (2000)
	J. Ilnytskyi *et al*., Phys. Rev. E 59, 4161 (1999).
Experiment:	
	G. S. Iannacchione *et al*. Phys. Rev. Lett. 71, 2595 (1993)
	X. Wu et al., Phys. Rev. Lett. 69, 470 (1992).

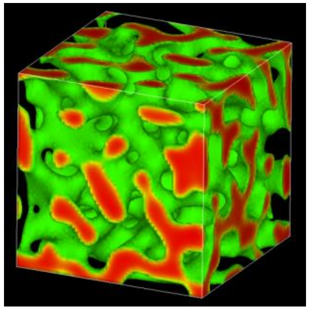
Nematic liquid crystal in porous media

The key point of our study is to deal with the structure of porous media more realistically.

This introduces the two important effects of the confinement.

1. topological constraint
2. surface anchoring



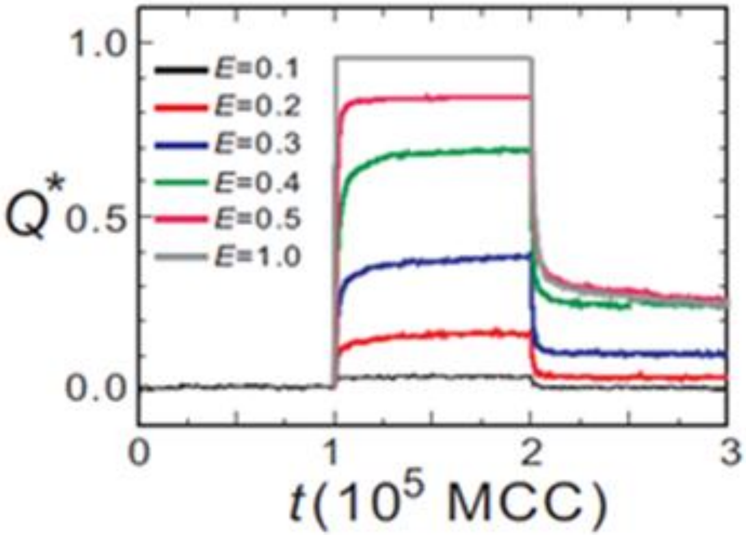


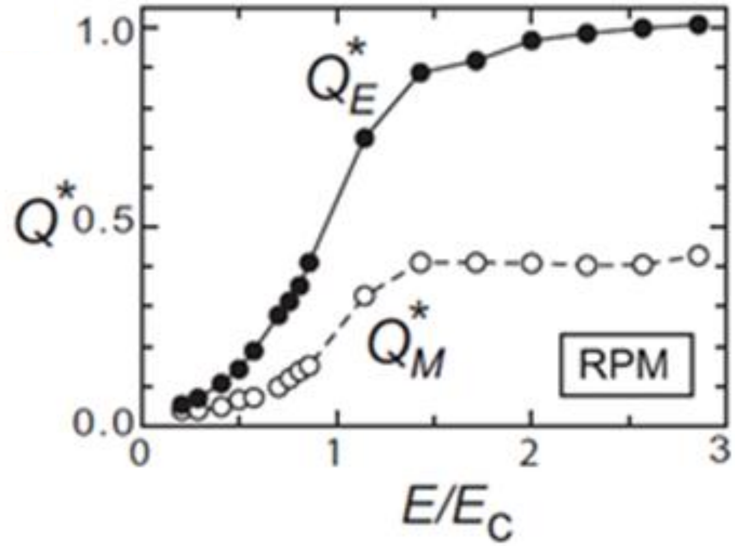
$$H = -\frac{1}{2} J \sum_{\langle i,j \rangle \in N \cup S} \left(\vec{n}_i \cdot \vec{n}_j \right)^2 - W \sum_{i \in S} (\vec{n}_i \cdot \vec{s})^2 - E^2 \sum_{i \in S \cup N} (\vec{n}_i \cdot \vec{z})^2$$

Induced and remnant nematic orders

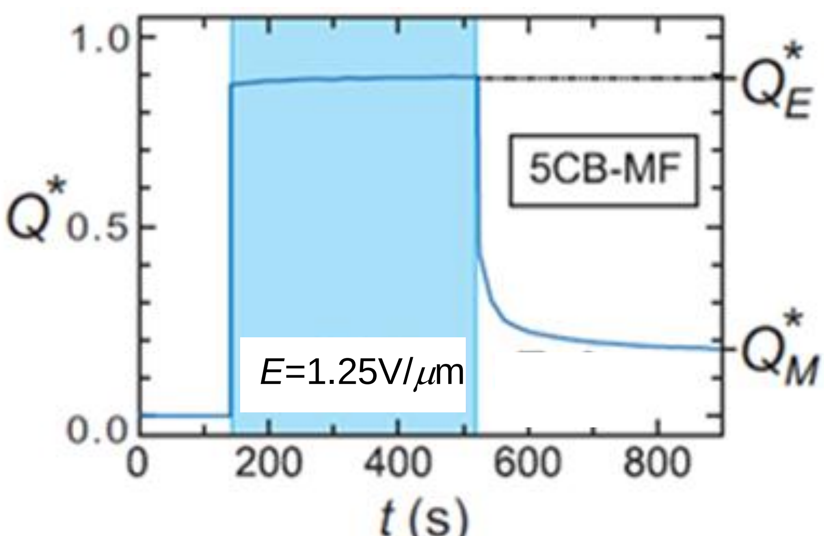
$Q^* = Q/Q_0(T)$

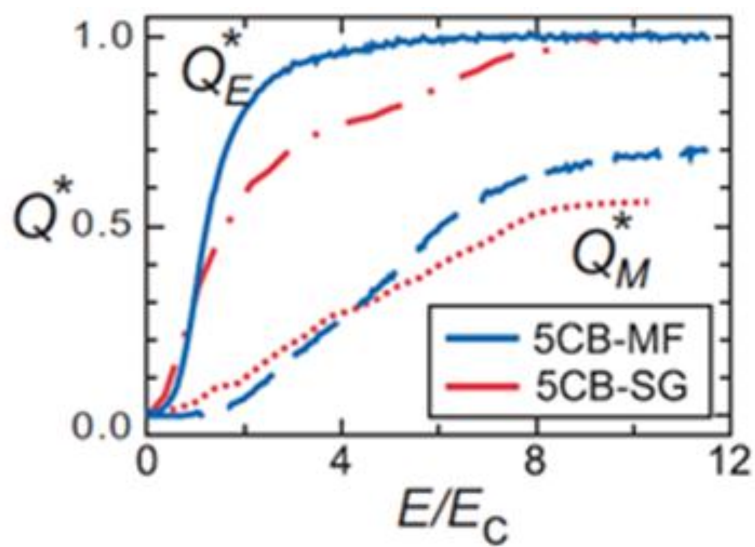
simulations



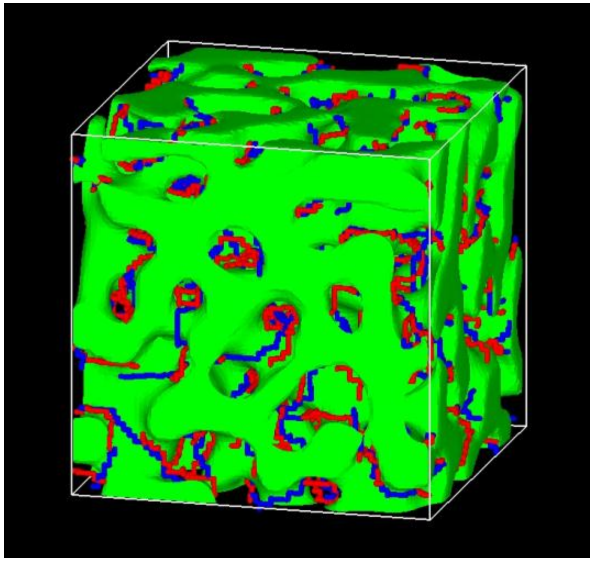


experiments (5CB in millipore filter (3μm) and silica gel (0.8mm))





Defect structure of nematic liquid crystal in porous media



defect structures for different simulations of the same condition

Since all the channels do not necessarily have disclination lines running through them, many metastable configurations can be found.

The defect configurations are long-lived since the energy barriers connecting them are much higher than thermal fluctuations.

This results in non-ergodic glassy behaviors, analogous to a spin glass.

The number of the possible configurations is estimated as, $(p-1)^{1-\chi/2}$

p average number of arms at nodes, typically $p \approx 3-6$

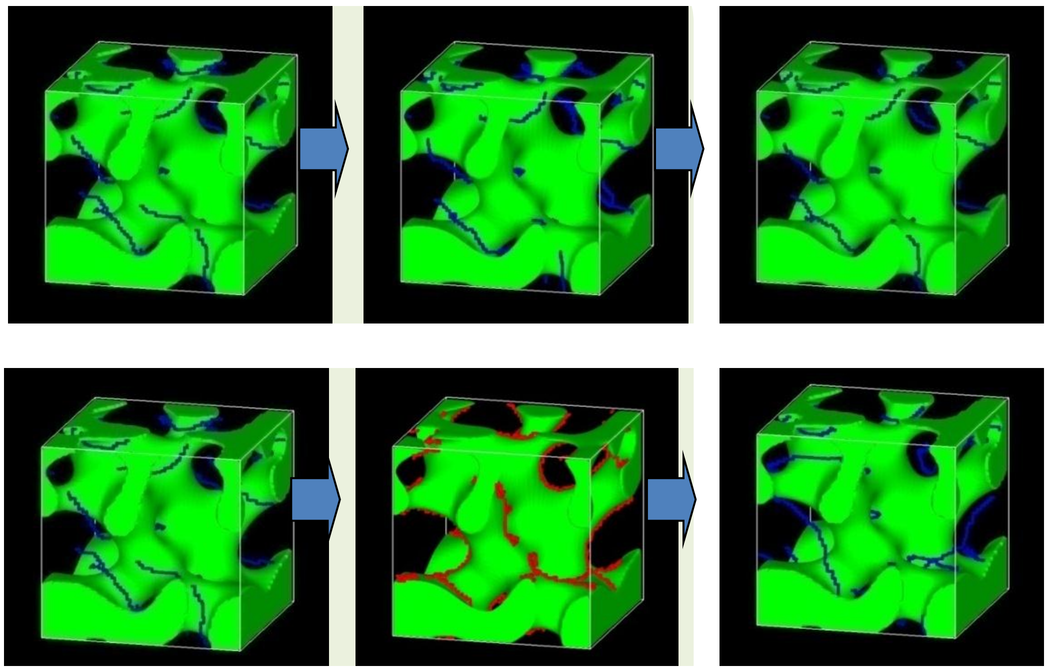
χ Euler characteristic (topological invariant) $\chi = \frac{1}{2\pi}\int dSK$

$\sim 10^{1000000}$ for 1 mm cell of 1μm pores !

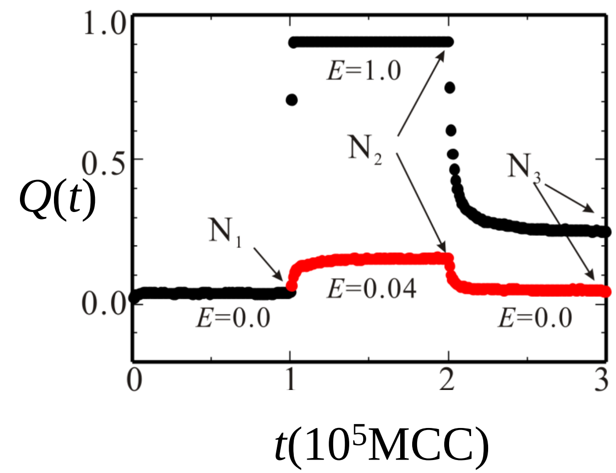
Transformation of defect structure by an external field

E=0.3

E=1.0



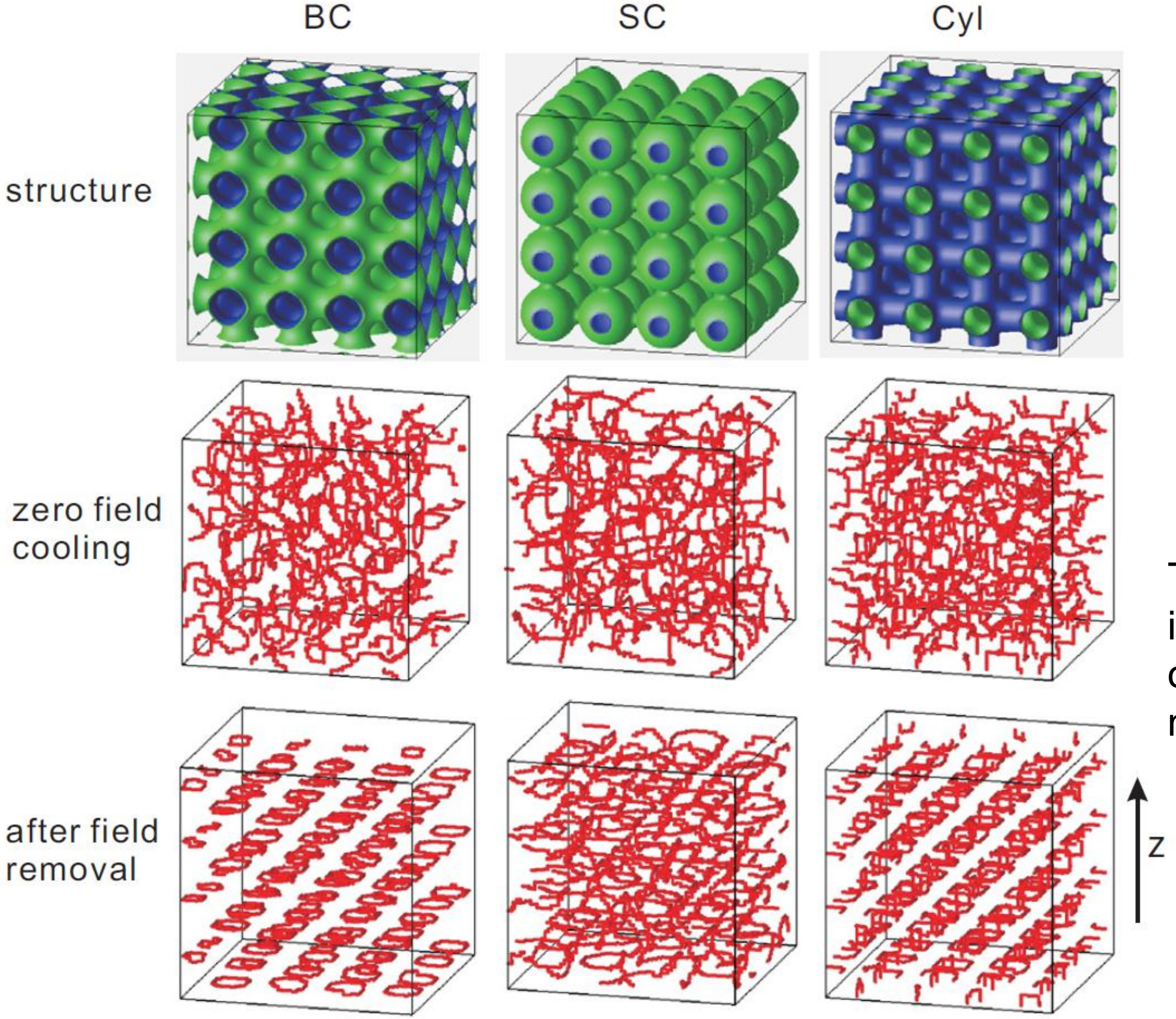
Before the quench under an electric field after the application



A strong field melts the defect structure and the topology of defect structure can be changed.

The new topology is conserved even after the field is switched off!

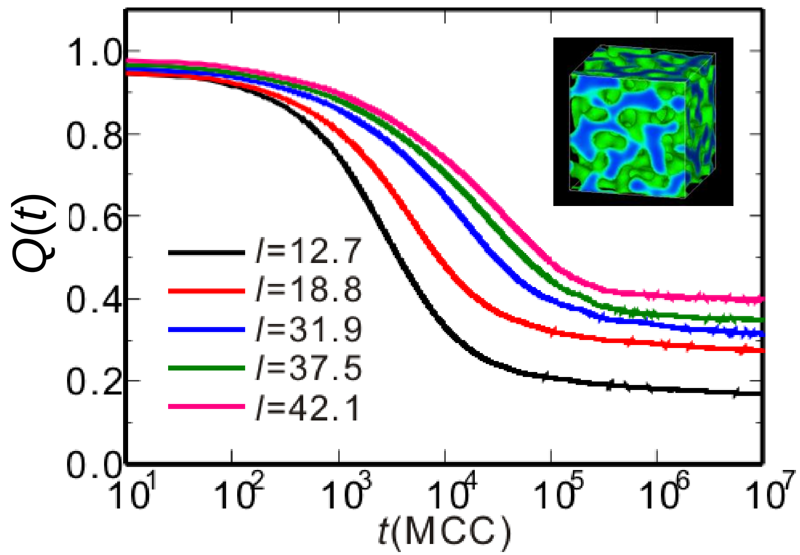
NLC in regular porous materials



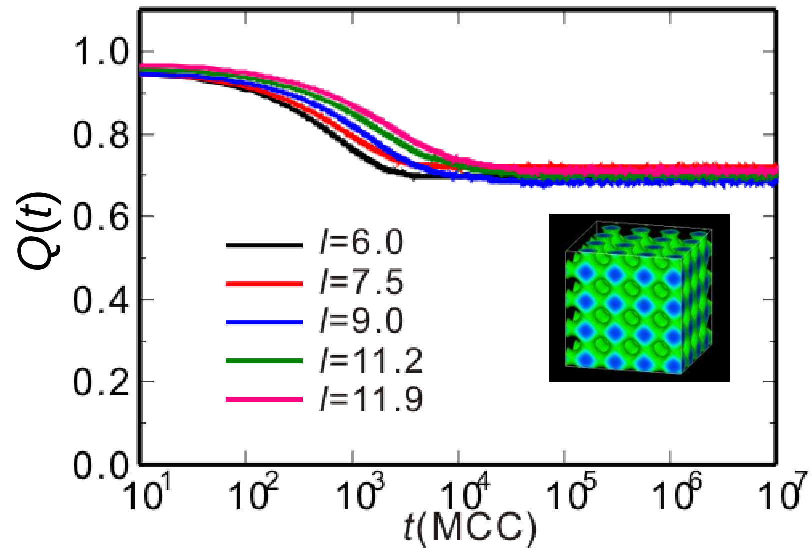
The defect structure is also regular in ordered porous media.

Relaxation of memorized order

Random porous medium (PPM)



Bicontinuous cubic (BC)



In BC, only a single relaxation mode is observed.
After the fast mode, the second slow relaxation appears in RPM.

BC: single stretched exponential decay

$$Q(t) = Q_M + \Delta Q_S \exp(-(t/\tau_S)^\alpha)$$

RPM: stretched exponential decay and logarithmic decay

$$Q(t) = Q_M + \Delta Q_S \exp(-(t/\tau_S)^\alpha) + \frac{\Delta Q_L}{1+\log(1+t/\tau_L)}$$

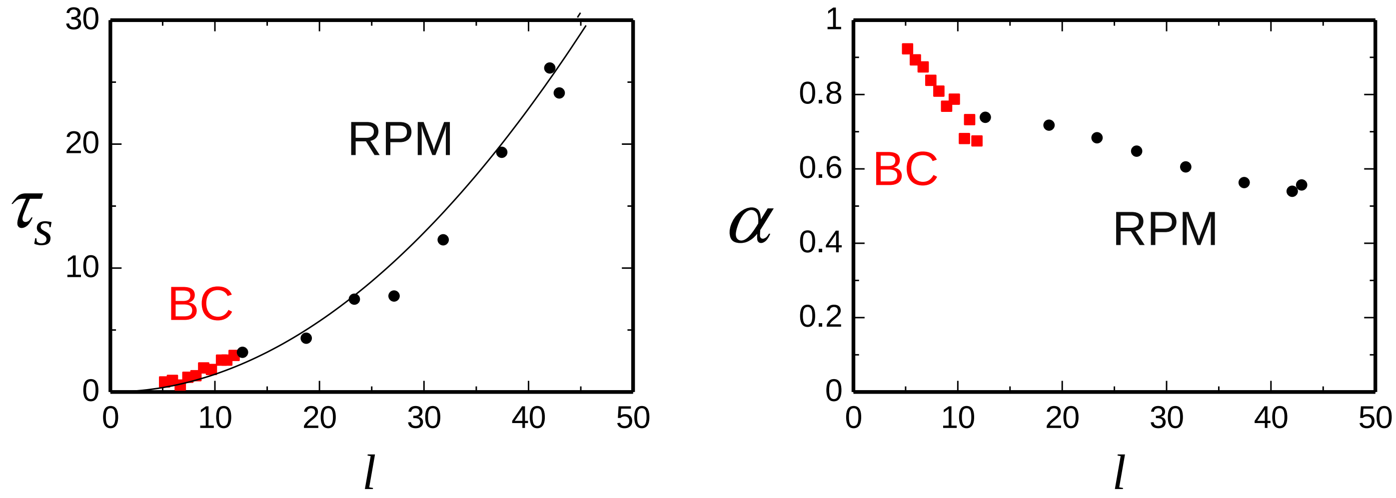
Logarithmic decay for superconductor:

P. W. Anderson, Phys. Rev. Lett. 9, 309 (1962)
Y. B. Kim *et al., Phys. Rev. Lett. 9, 306* (1962)

Fast relaxation mode

In the both type of porous media, the fast relaxation mode represents the recovery of the distorted director field owing to the elasticity.

In this fast process, the topology of the defect structure does not change.



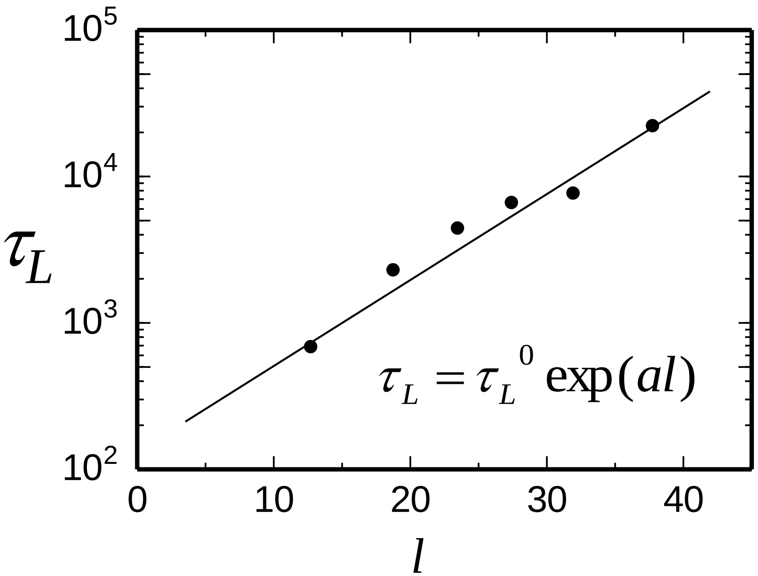
A continuum theory $$F\{\vec{n}\} = \frac{1}{2}K\int dV\left|\nabla\vec{n}\right|^2 + W\int dS\left(\vec{n}\cdot\vec{s}\right)^2 + \Delta\varepsilon\int dV(\vec{E}\cdot\vec{n})^2$$

$$\frac{\partial}{\partial t}\vec{n} = -\frac{1}{\nu}\frac{\delta F}{\delta\vec{n}} \quad \Rightarrow \quad \tau_s = \frac{\nu l^2}{K}$$

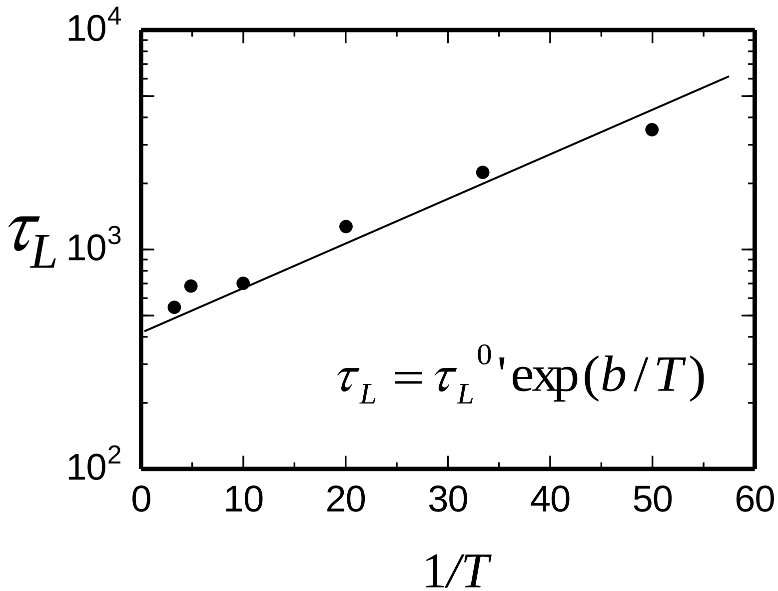
The second slow relaxation in RPM

$$Q(t) = Q_M + \Delta Q_S \exp(-(t/\tau_S)^{\alpha}) + \frac{\Delta Q_L}{1+\log(1+t/\tau_L)}$$

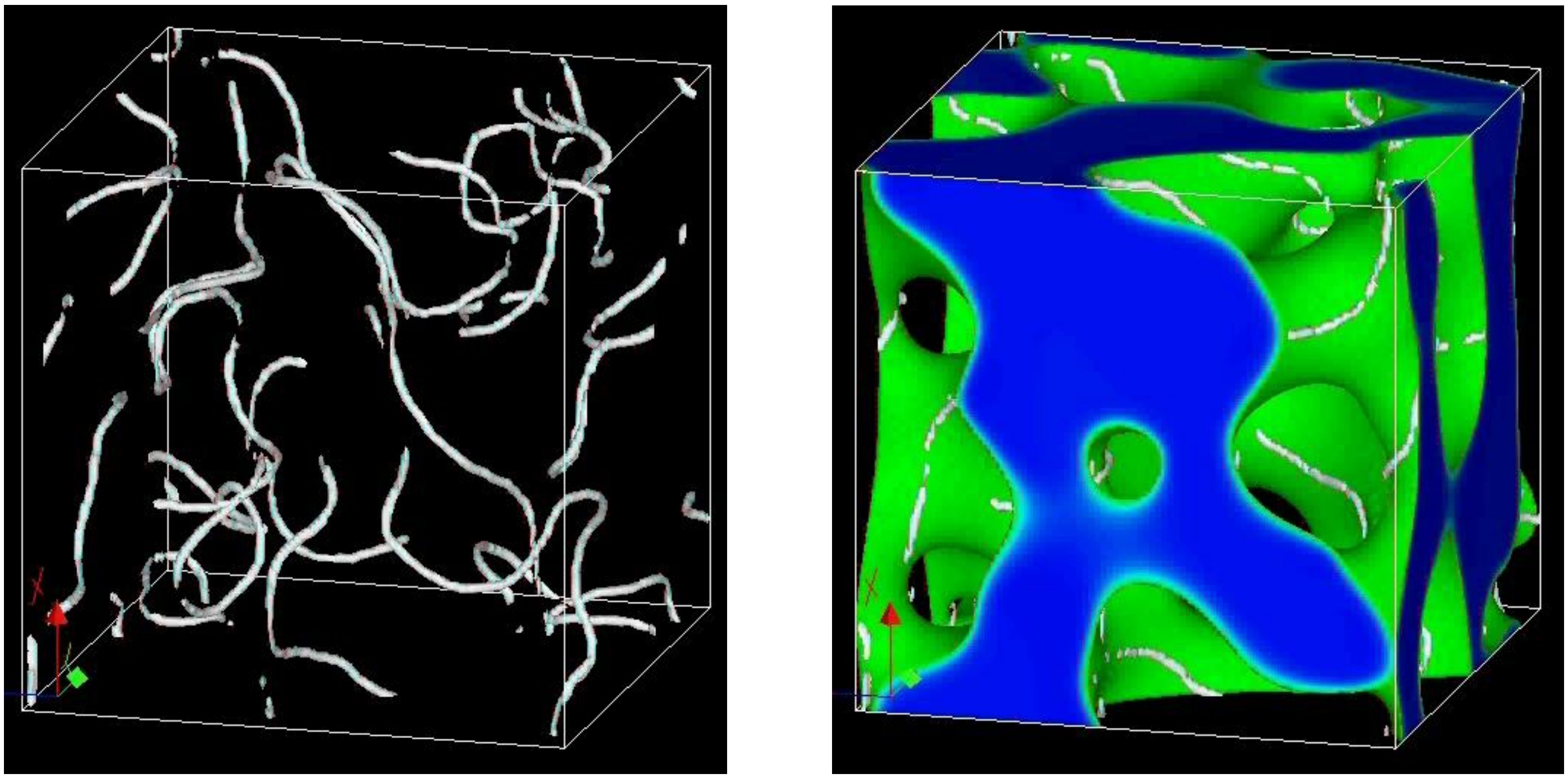
Pore size l –dependence at T=0.1



Temperature dependence for l=12.7



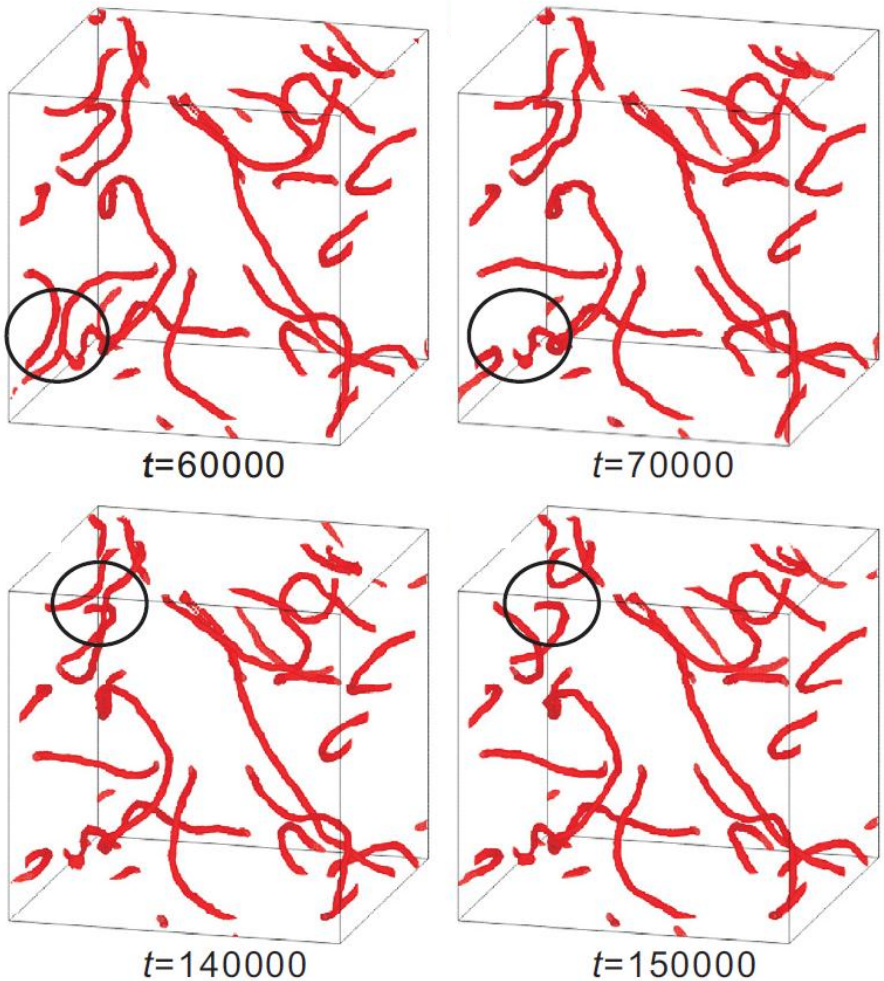
The topological change of the defect structure in RPM



At T=0.1 for l=43.9

The second slow relaxation accompanies the change of the topology of the defect structure.

The topological change of the defect structure in RPM



In a subunit of the volume l^3, the elastic energy density is estimated as

$$e = \frac{1}{2} K (\nabla \vec{n})^2 \sim \frac{1}{2} \frac{K}{l^2}$$

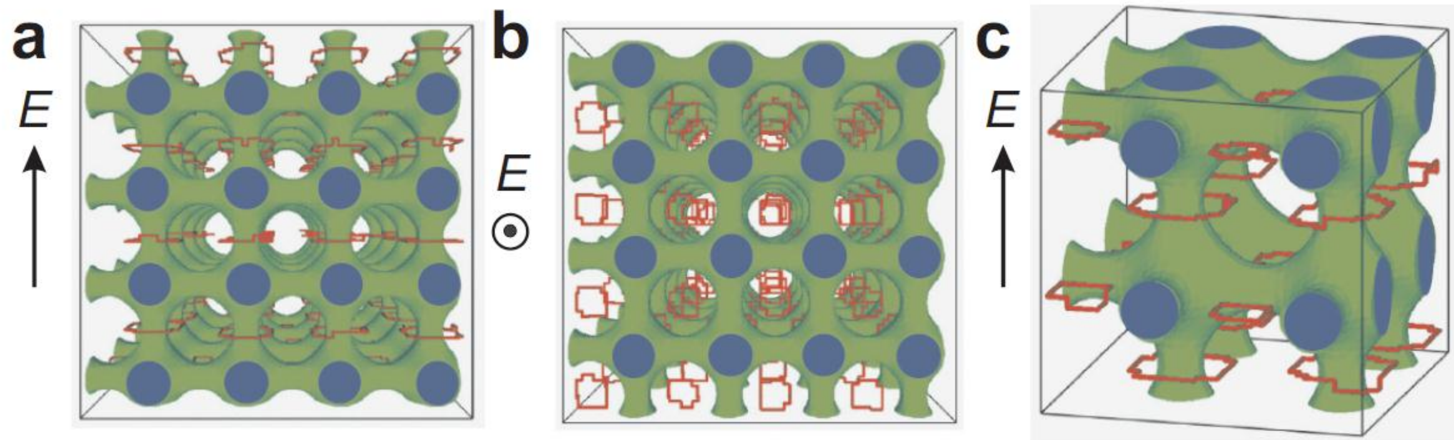
Thus, the stored elastic energy in this small volume is

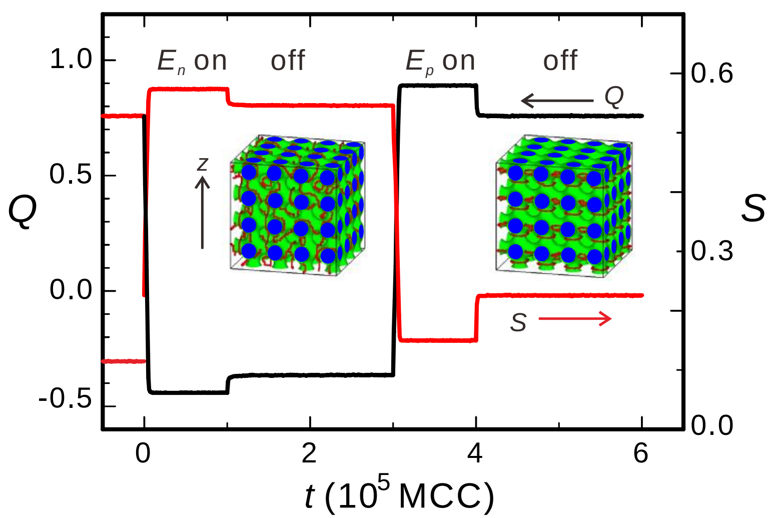
$$E = el^3 \propto Kl$$

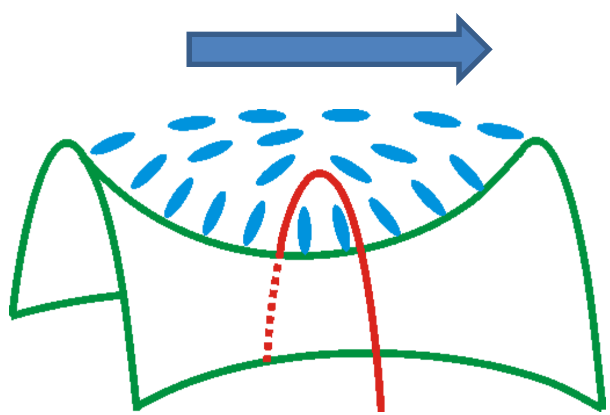
The energy barrier against the topological change is also scaled as Kl

$$\tau_L \propto \exp(cKl / T)$$

Defect pattern in a regular matrix

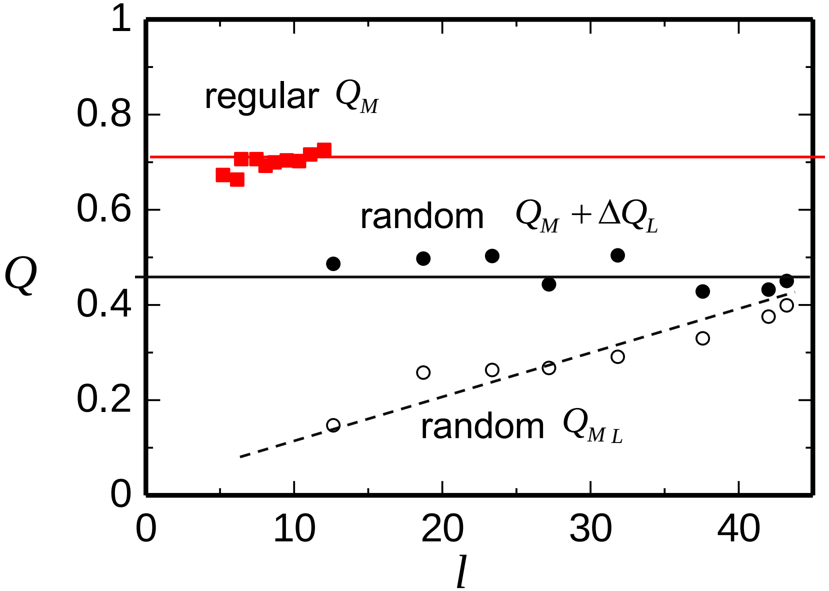


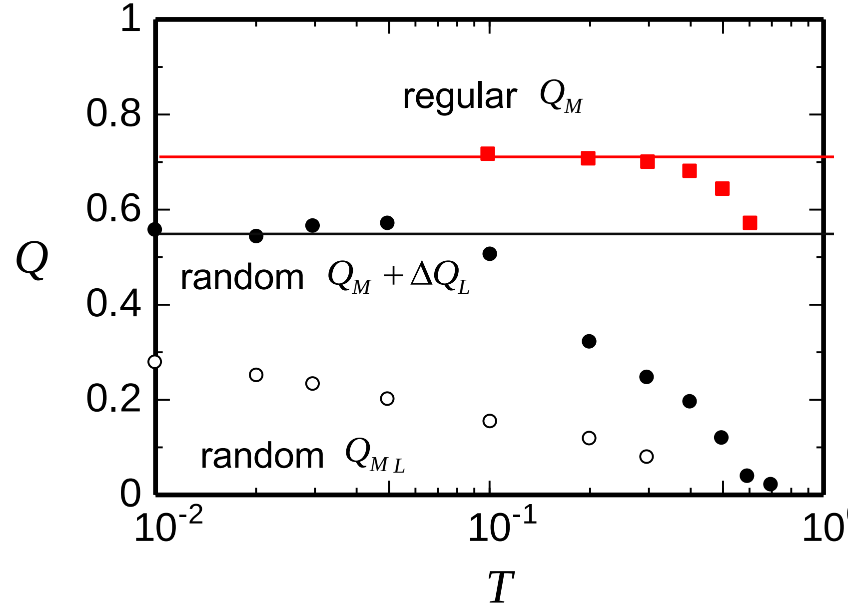




In a regular matrix, the defect structure reaches one of the most stable configuration after the fast mode. Then, the second mode is absent.

T and l - dependences of the remnant orders





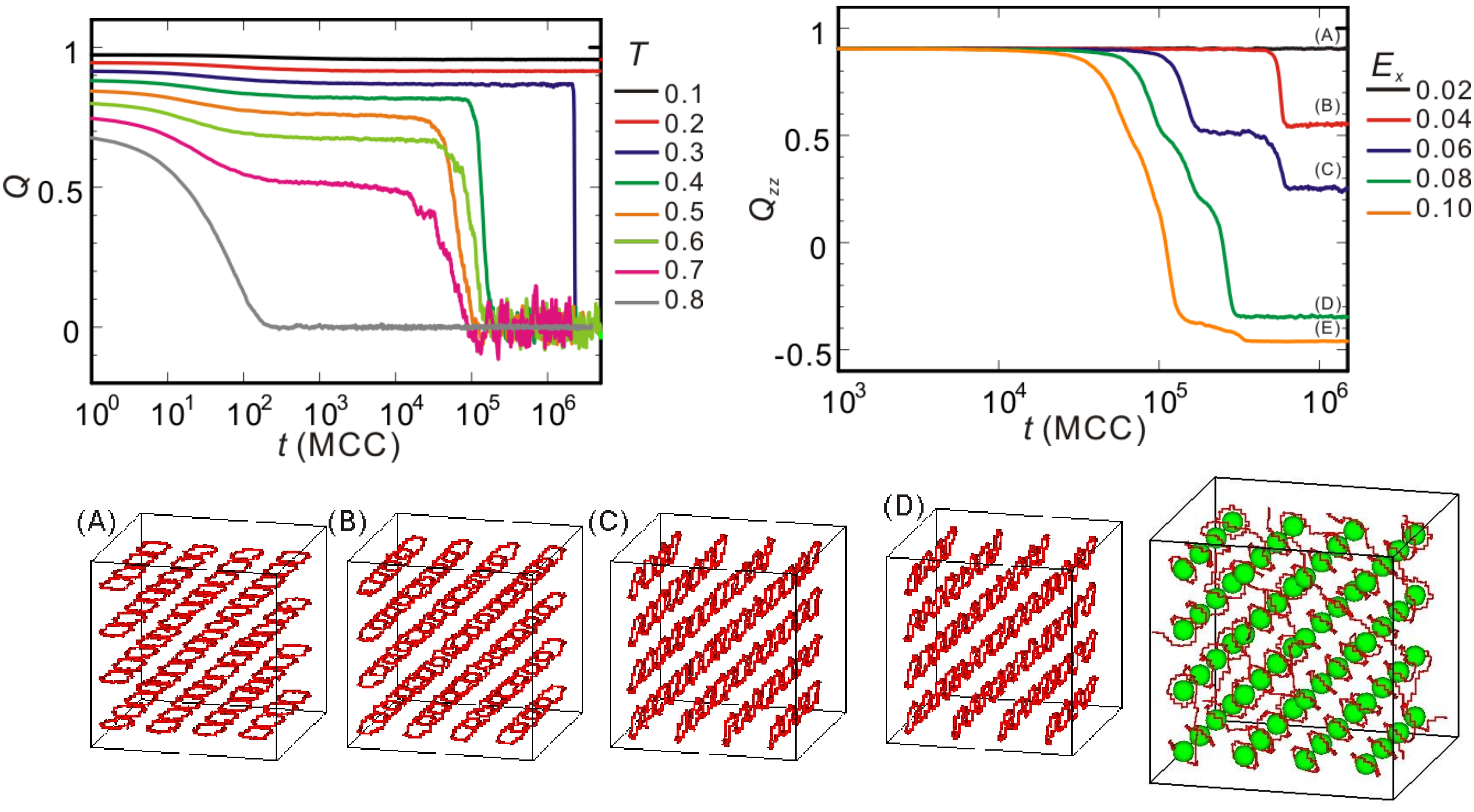
BC: $Q(t) = Q_M + \Delta Q_S \exp(-(t/\tau_S)^{\alpha})$

RPM: $Q(t) = Q_M + \Delta Q_S \exp(-(t/\tau_S)^{\alpha}) + \dfrac{\Delta Q_L}{1+\log(1+t/\tau_L)}$

In a regular matrix, the remnant order appears to be independent of the pore size. This is consistent with the scaling argument for the strong anchoring case.

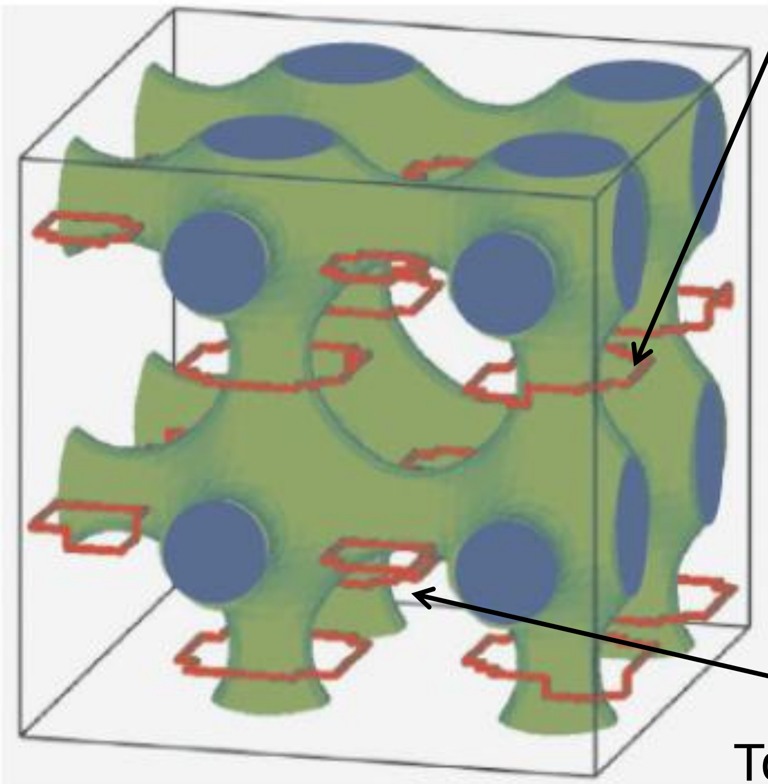
In an irregular matrix, the remnant depends apparently on the mean pore size because of its non-ergodic glassy behavior.

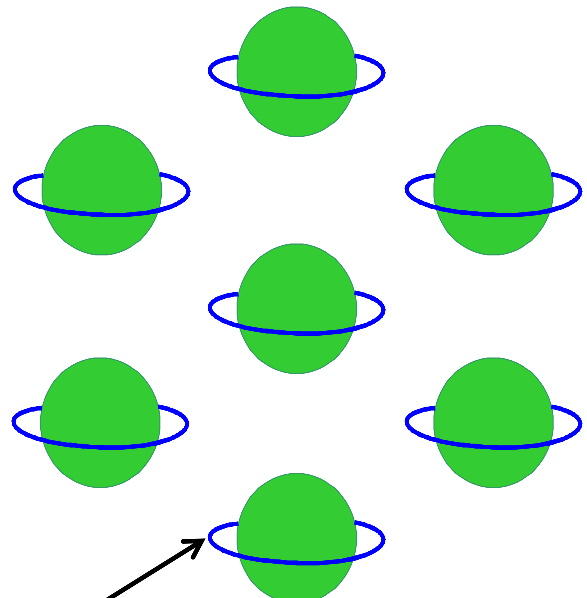
Relaxations without reconfigurations of defects



Roles of the connectivity of topological defects

Topologically locked defect





Topologically free defect

Changes of the director pattern in a bicontinuous medium should accompany reconfiguration of the defects.

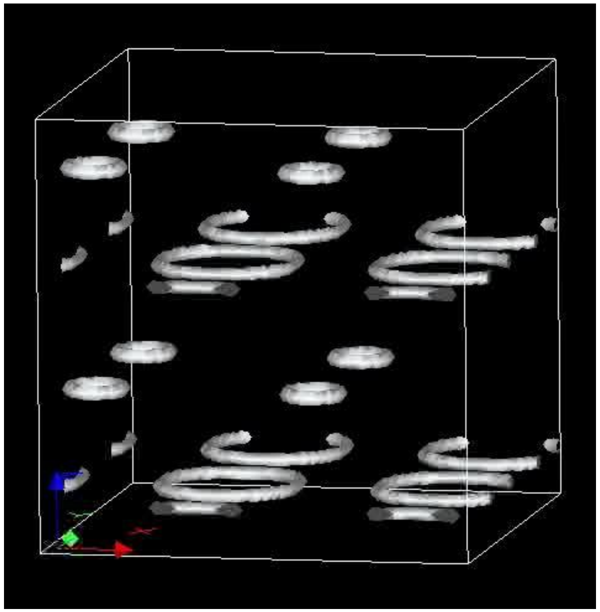
Such changes ares strongly suppressed because the energy barrier for them is very high ($\sim 10^3\, k_B T$)

Similarity and difference

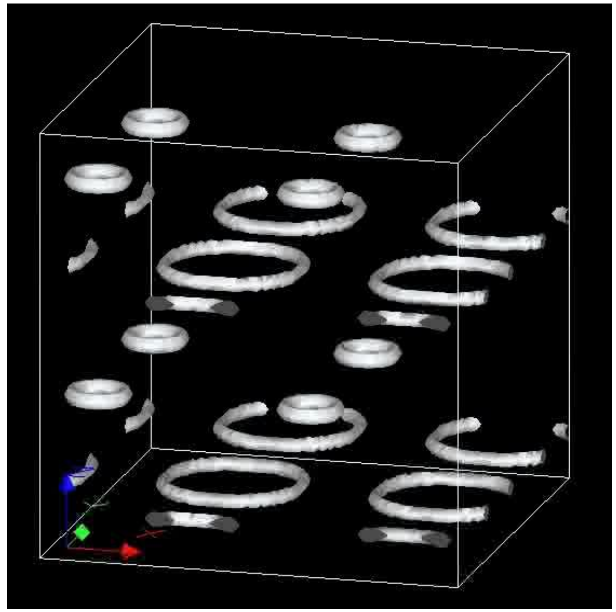
	nematic	electrostatic
(free) energy	$F=\frac{K}{2}\int d\vec{r}\left(\nabla\vec{n}\right)^2$	$F=\frac{\varepsilon}{8\pi}\int d\vec{r}\,\lvert\nabla\Phi\rvert^2$
Interaction potential	$V(r)\sim\frac{ss'}{r}$ (in the far field)	$V(r)\sim\frac{ZZ'e^2}{r}$
annihilation	$s+(-s)\rightarrow 0$	$e^{+}+e^{-}\rightarrow\gamma+\gamma$
symmetry	$\vec{n}\sim-\vec{n}$	$\Phi\neq-\Phi$
singularity	point defect line defect (disclination)	point defect (electric charge)

Interaction mediated by disclinations
depends on the topology of the defects

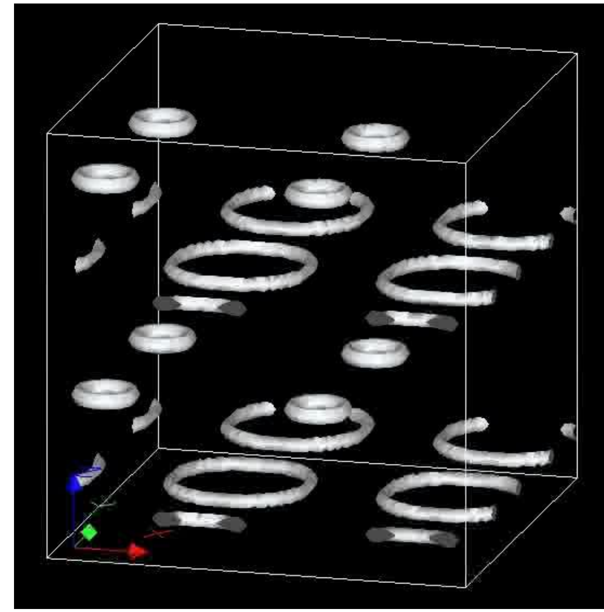
Flow directed along the director field



$F_z = 0.003$



$F_z = 0.004$



$F_z = 0.005$

If an intermediate force is applied ($0.003 <= F_z <= 0.004$), the unlocked defect rings move along the flow. When the moving distance reaches to be comparable to the pore unit length, the defect disappears and a new defect is created almost at the original position. This cycle is repeated with frequency proportional to the flow speed.

When a strong flow is imposed, the locked defects are also destroyed.

Summary

We numerically study roles of connectivity of topological defects of nematic liquid crystals in complex geometries.

When a nematic liquid crystal is confined in a porous medium or contains solid objects as a host liquid, coupling of the director to the solid surface may easily conflict with the symmetry of the ordered phase and thus lead to frustration and topological defects.

Reflecting the topology of space filled with a nematic liquid crystal, there remain many defects with a large number of possible configurations. Since there exist energy barriers much higher than the thermal energy among the meta-stable defect configurations, reorganization of the director field with accompanying the topological changes of the defects is strongly suppressed.

Such suppressed reorganization leads to interesting non-ergodic behaviors in nematic liquid crystals.

The origin of the logarithmic slow decay

The rate of the change in the remnant order is assumed to be

$$\frac{\partial Q_M}{\partial t} = -A\exp\left\{\frac{\Delta U(Q_M)}{k_B T}\right\}$$

Assuming the change in Q_{M} is through that in U, we obtain

$$\left(\frac{d\Delta U}{dt}\right) = \left(\frac{d\Delta U}{dQ_M}\right)\left(\frac{dQ_M}{dt}\right) = -A\left(\frac{d\Delta U}{dQ_M}\right)\exp\left\{\frac{\Delta U(Q_M)}{k_B T}\right\}$$

$$\Rightarrow \quad \Delta U(Q_M) = k_B T \ln(t/t_0) \qquad\qquad t_0 = k_B T/\{A(d\Delta U/dQ_M)\}$$

The simplest expression for the barrier is linearly decreasing function of Q_{M}

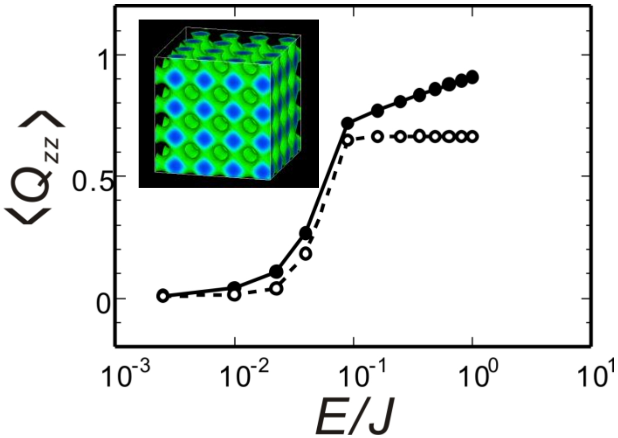
$$\Delta U = U_0\left[1 - \frac{Q_M}{Q_0}\right]$$

$$\Rightarrow \quad Q_M(t) = Q_0\left[1 - \frac{k_B T}{U_0}\ln\left(\frac{t}{t_0}\right)\right]$$

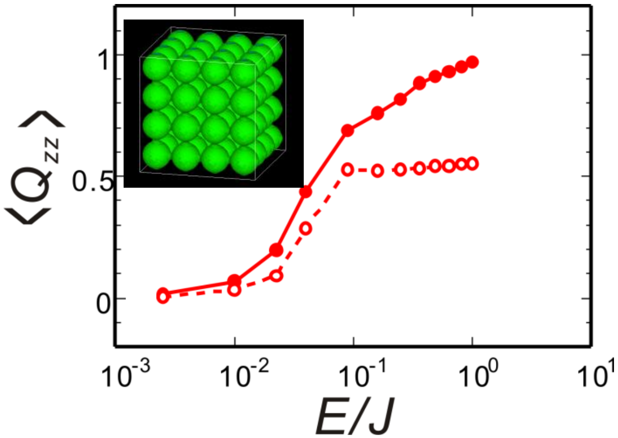
P. W. Anderson, Phys. Rev. Lett. 9, 309 (1962)
Y. B. Kim *et al., Phys. Rev. Lett. 9, 306* (1962)

Memory effect of nematic liquid crystal in porous media

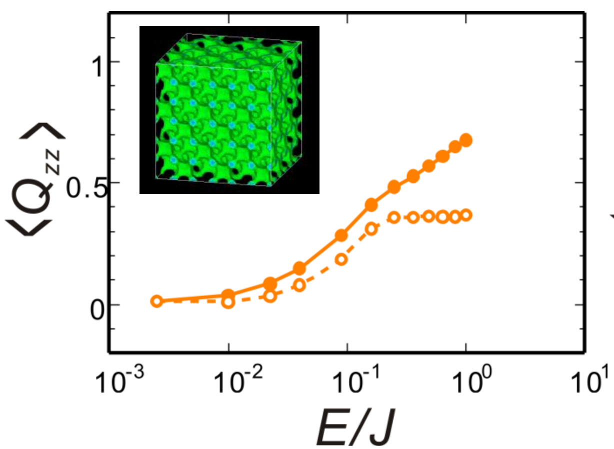
bicontinuous cubic



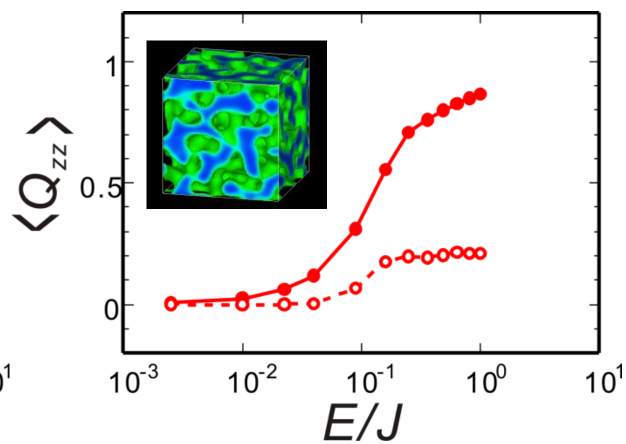
SC sphere array



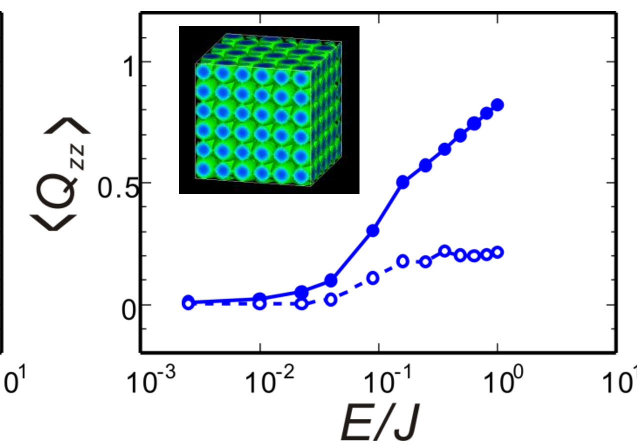
inverted FCC sphere array



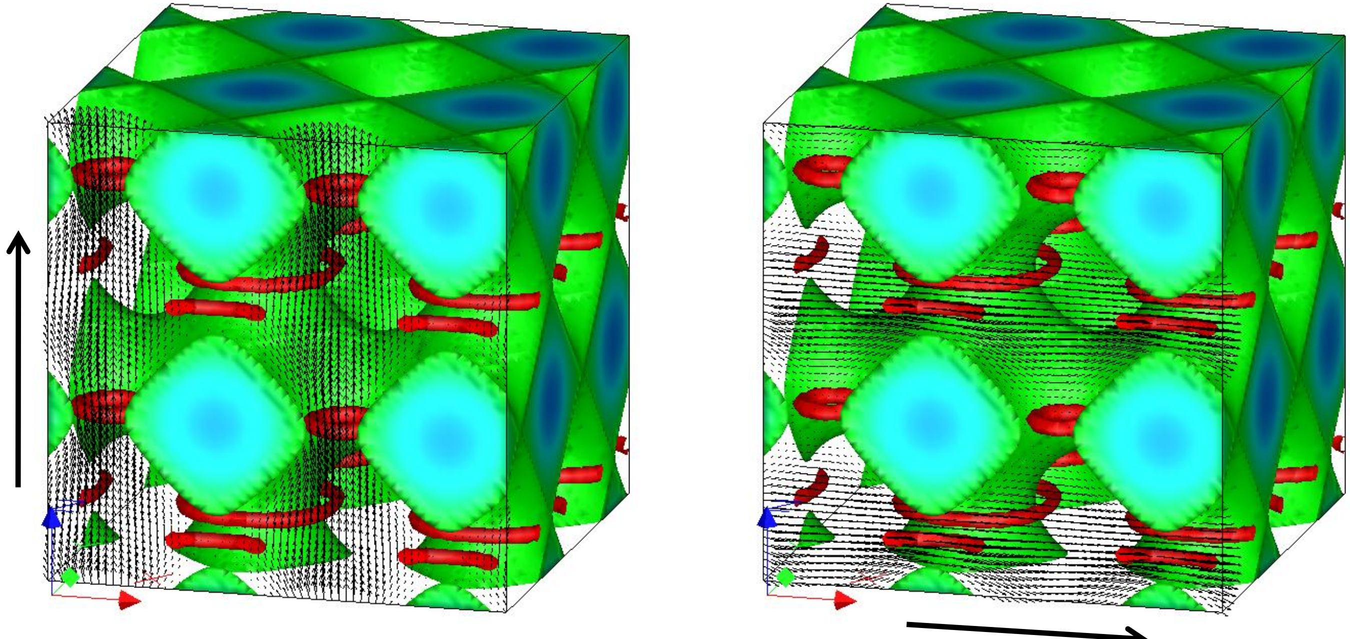
random pores



FCC sphere array



Effect of flow on the director field in porous media



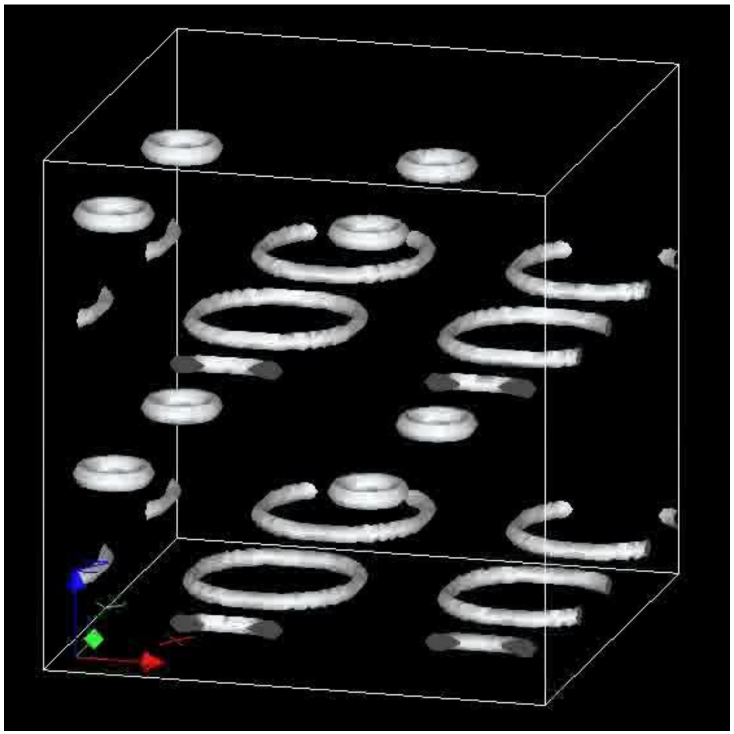
$F_z = 0.0004$ $F_x = 0.0004$

Lattice Boltzmann simulation of nematohydrodynamics in complex geometry

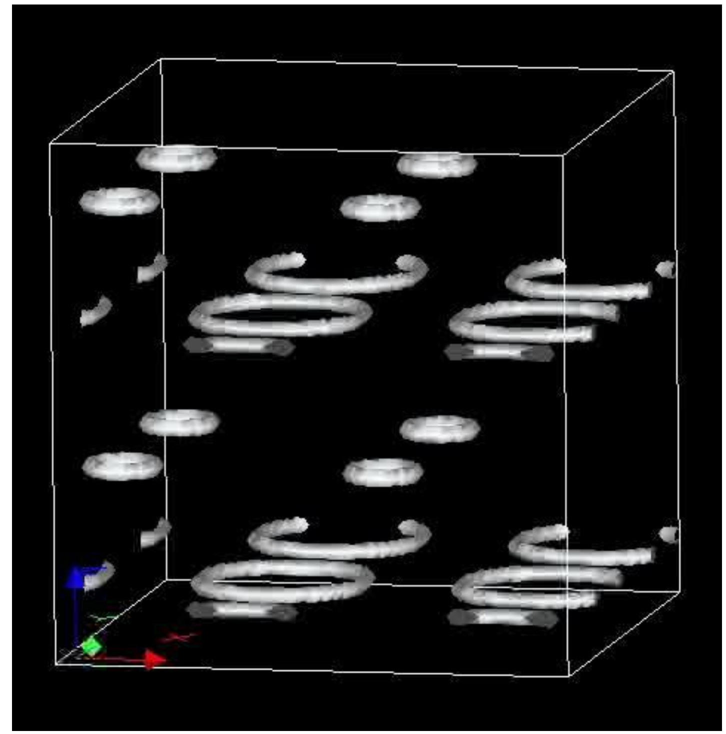
C. M. Care *et al*., Phys. Rev. E. 67, 061703 (2003).
C. Denniston et al., Europhys. Lett. 52, 481 (2000).
S. Succi, *The Lattice Boltzmann Equation for Fluid Dynamics and Beyond* (2001)

T. Araki, in preparation

Flow directed along the director field



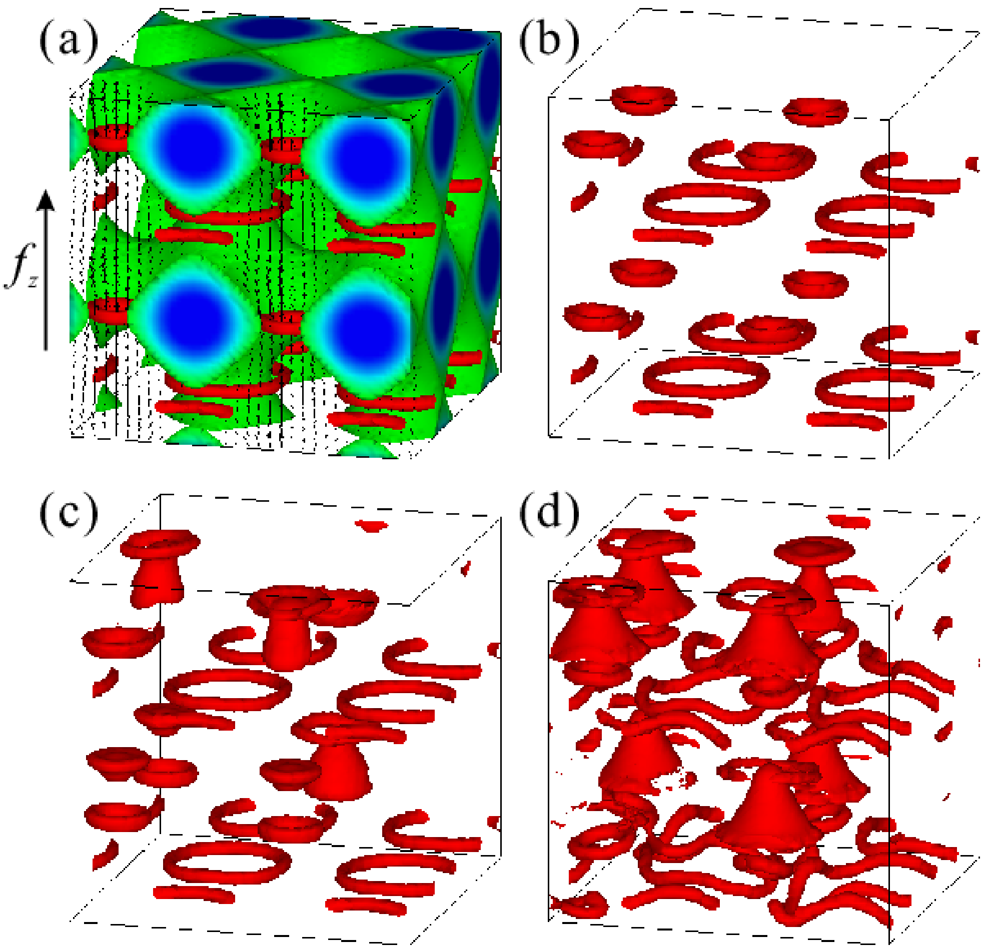
$F_z = 0.001$

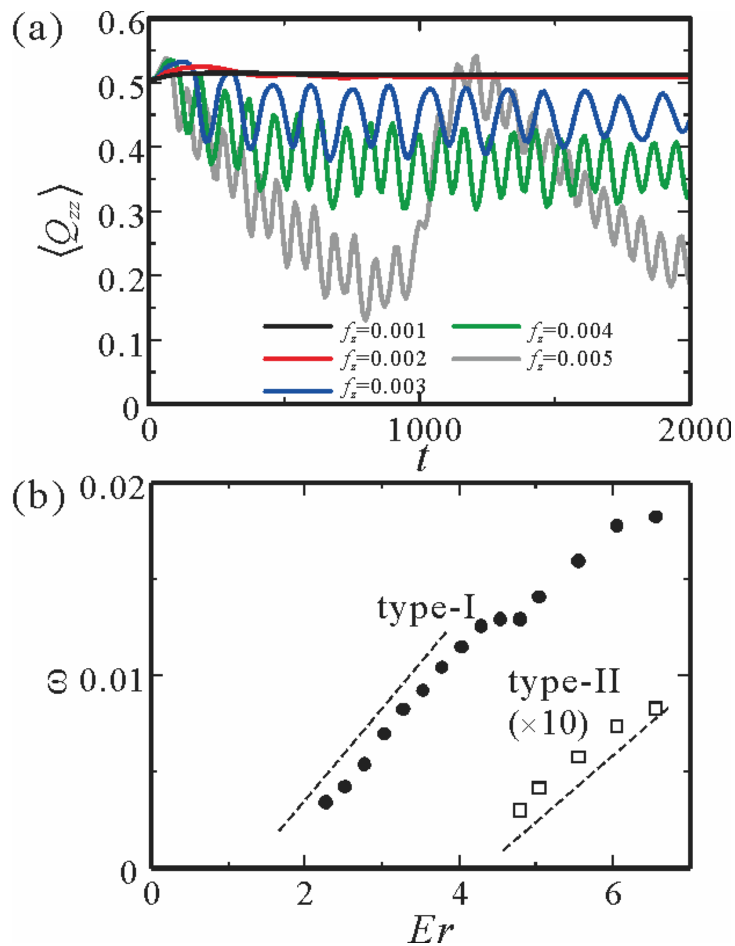


$F_z = 0.002$

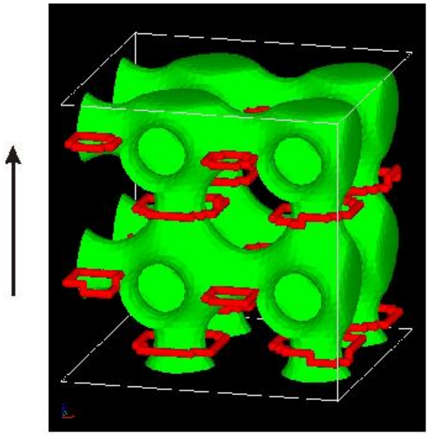
For a weak external stress (F_z<=0.002), the disclination lines are slightly distorted without topological changes.

Flow directed along the director field



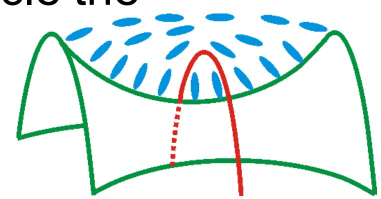


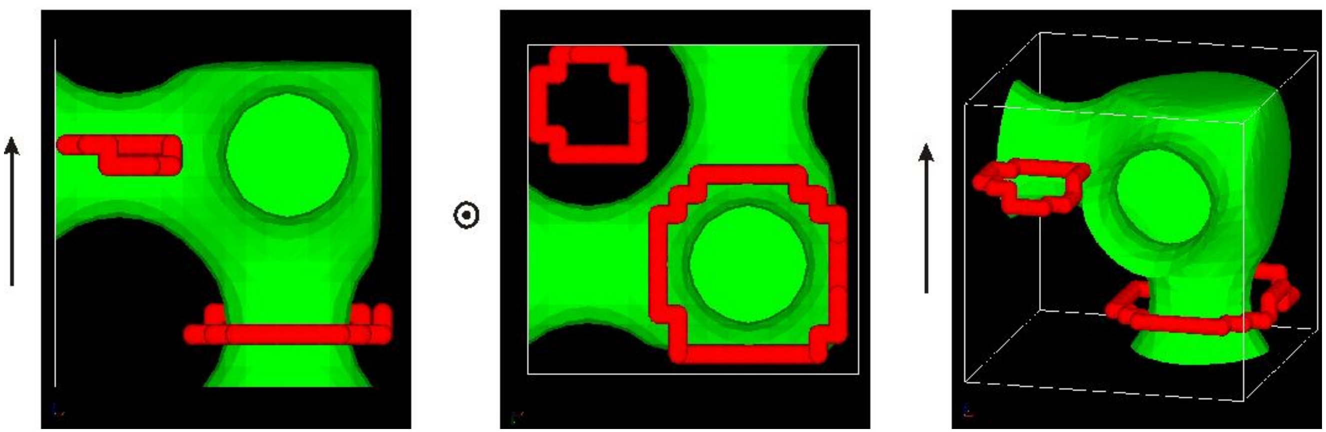
Defect structures in bicontinuous cubic



There remains two types of defect rings.

Half of the disclination lines with $s=1/2$ encircle the neck of the pores.
Others ($s=-1/2$) are surrounded by neighboring nodes and necks.
And they are aligned perpendicularly to the field.

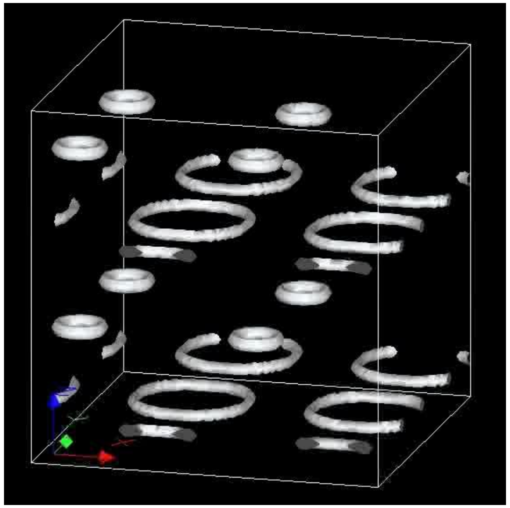




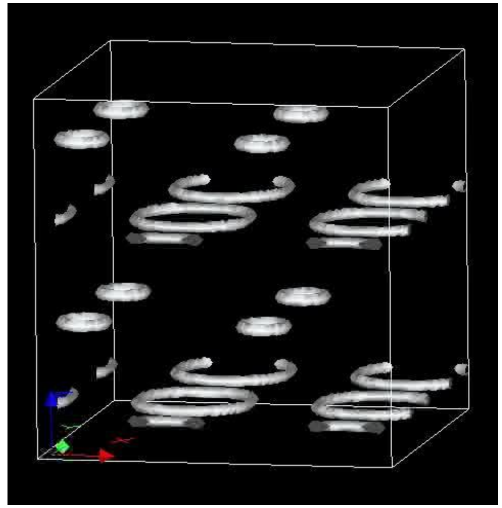
The total amount of the defect charges is related to Gaussian curvature

$$\sum_i s_i = 1 - g$$

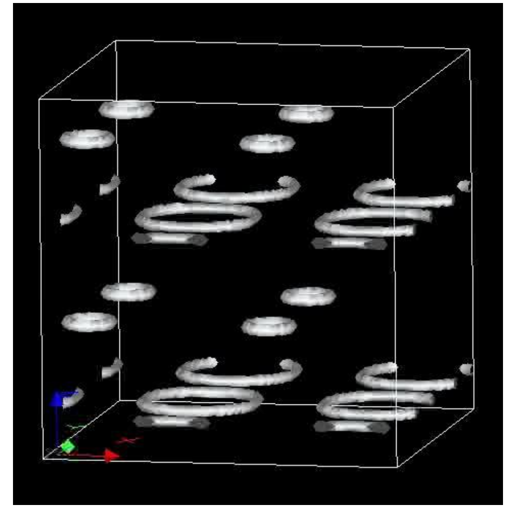
Flow perpendicular to the director field



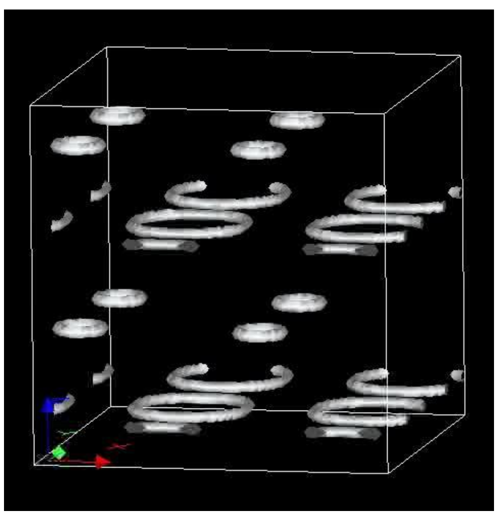
$F_x = 0.001$



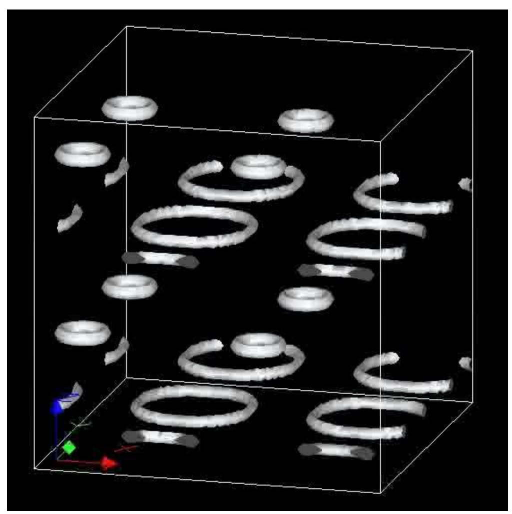
$F_x = 0.002$



$F_x = 0.003$

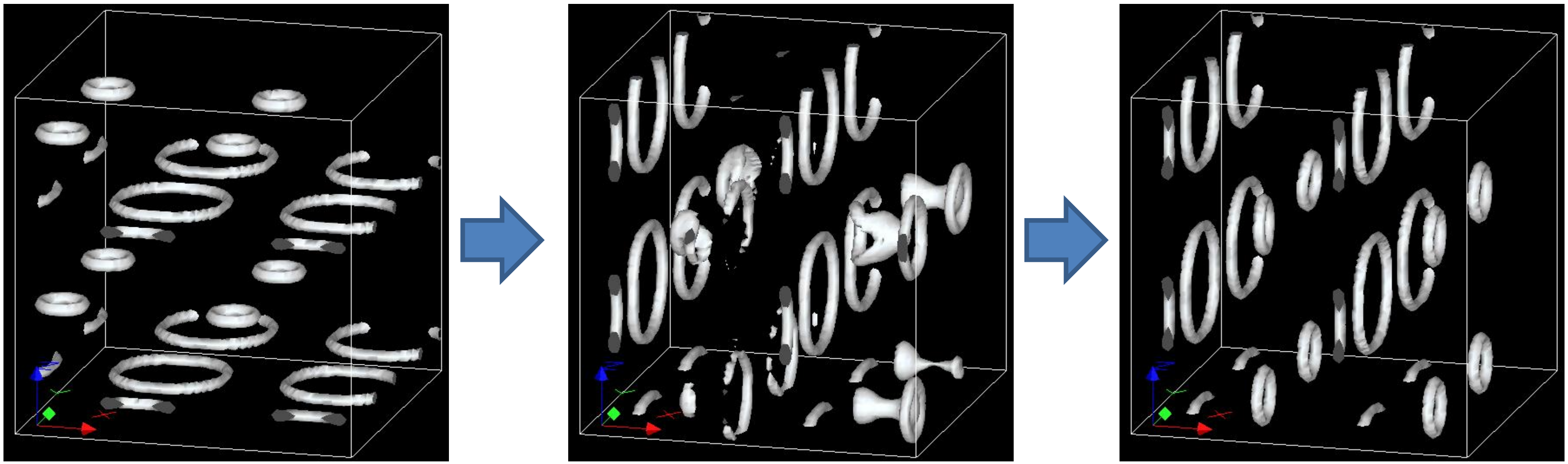


$F_x = 0.004$

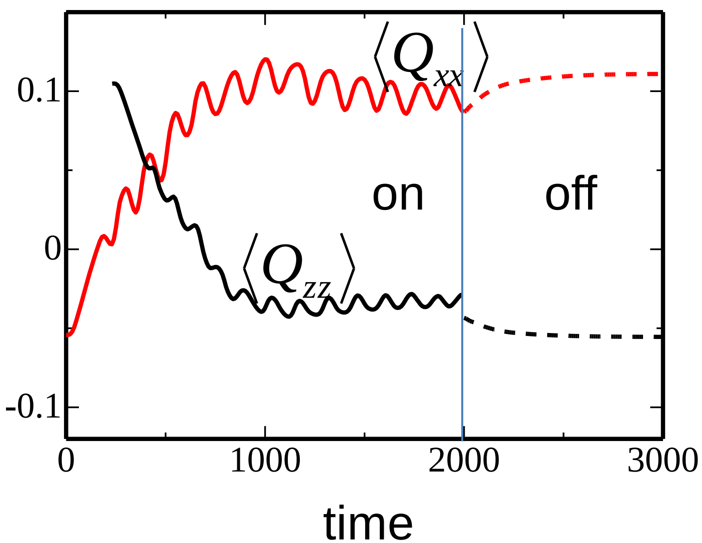


$F_x = 0.005$

Flow perpendicular to the director field



$F_x = 0.003$



A flow can also switch the memory of the director field!

Flow perpendicular to the director field