Presented at the COMSOL Conference 2010 China

Study of ER Non-equilibrium Behavior with COMSOL

Cong LI and Luwei ZHOU
Physics Department, Fudan University
Shanghai 200433, P.R.China
lwzhou@fudan.edu.cn

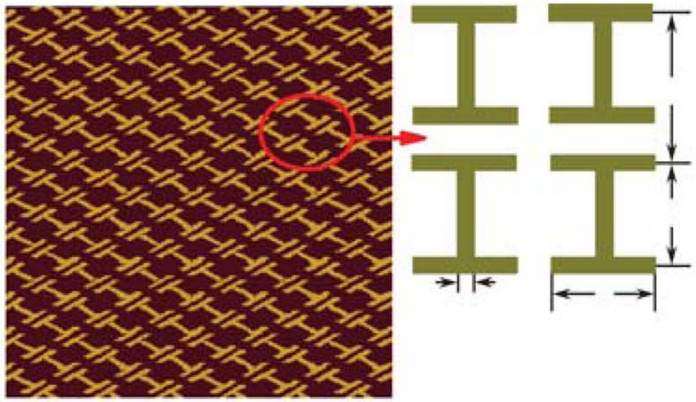
1. Theory -

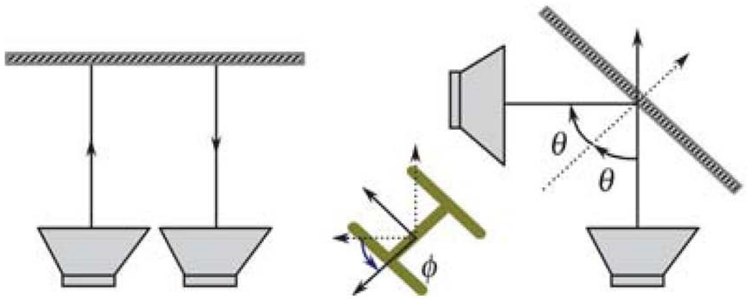
COMSOL: A powerful tool in theoretical study

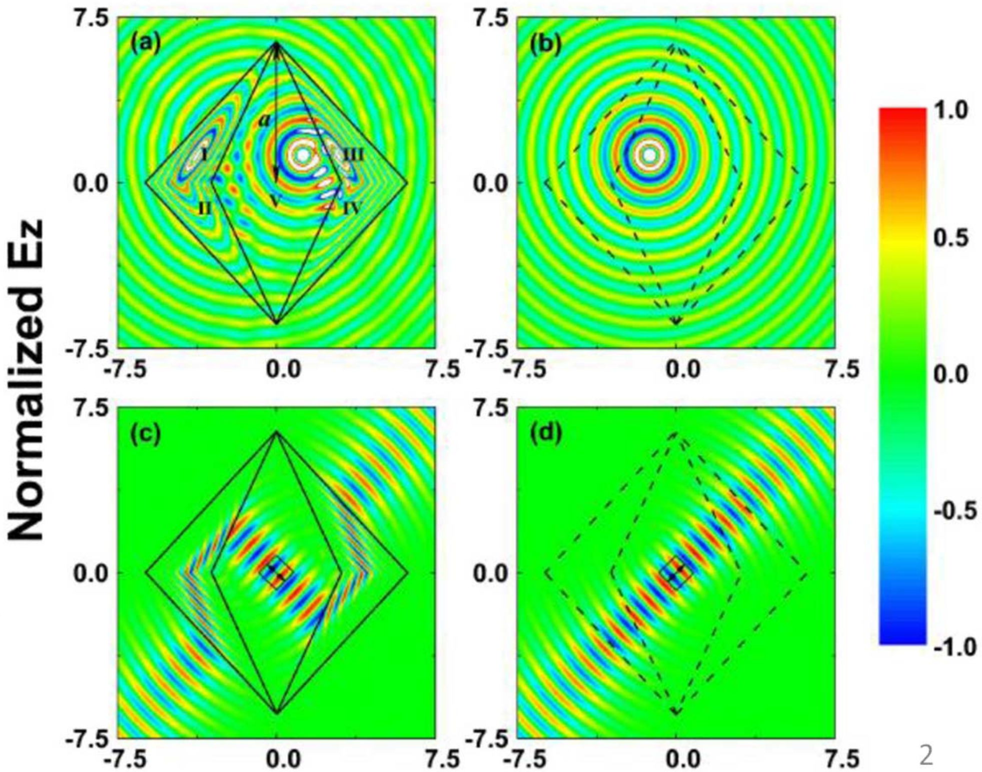
Lei ZHOU et al.,
Physics Department, Fudan University.

Metamaterials:

Microwave → **Visible light**

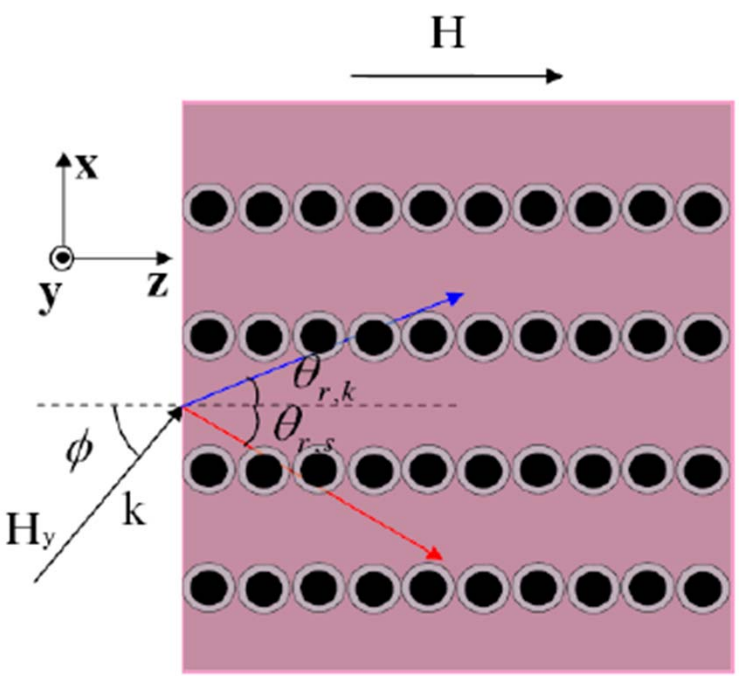






Negative refraction indices

Jiping HUANG et al., Fudan University.



Three factors:

1. Metal core or shell
2. Form chains or columns
3. Lamella

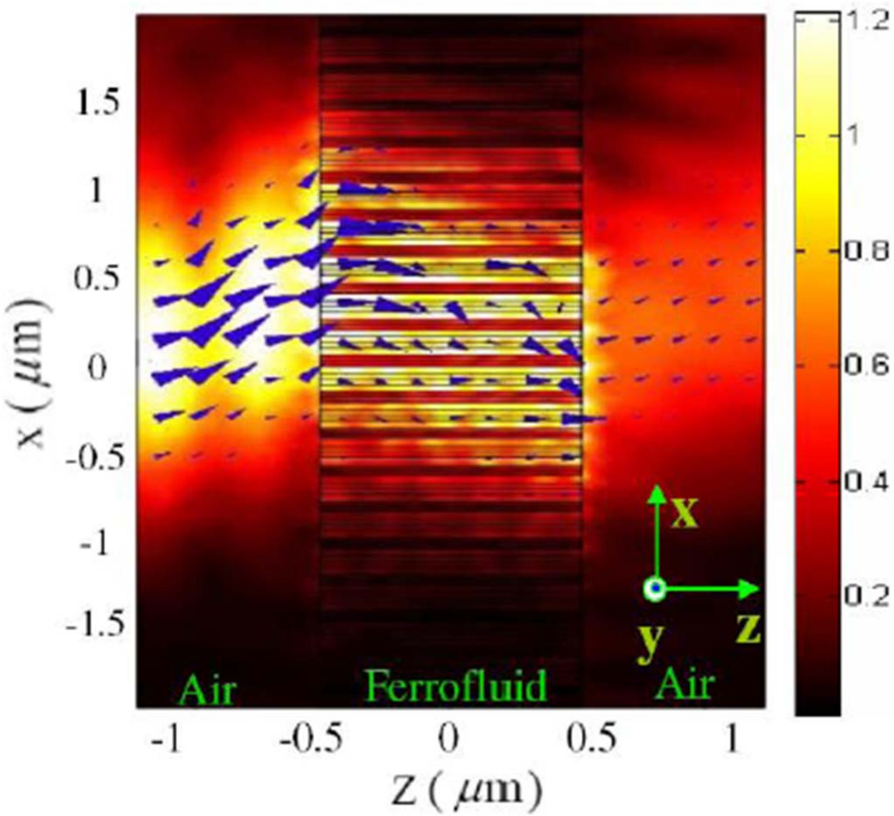
Y. Gao, et al., PRL 104, 034501 (2010)

Hard → **Soft** metamaterials

Single frequency → Broad band frequencies

Optic Invisibility → **Acoustic** Invisibility

Wavelength 758nm 3D



Y. Gao, et al., PRL 104, 034501 (2010)

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In the January 30 Issue:

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LIQUID LIGHT BENDER PROPOSED

Tiny nanoparticles dispersed in fluid may hide objects

By Laura Sanders
Web edition : Thursday, January 14th, 2010

Text Size

Tiny silver-coated rust particles suspended in water may give the fluid light-bending superpowers, physicists suggest in a paper to appear in *Physical Review Letters*.

Simulations with the proposed fluid system find that it could disguise objects from many wavelengths of visible light, lead author Jiping Huang of Fudan University in Shanghai and colleagues report. What's more, the system would be tunable, giving researchers control over the light-contorting particles.

The ability to twist and contort light in unusual ways has been demonstrated in a special class of materials called metamaterials. New metamaterial designs may

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How to make a liquid invisibility cl

14:51 08 January 2010 by Kate McAlpine

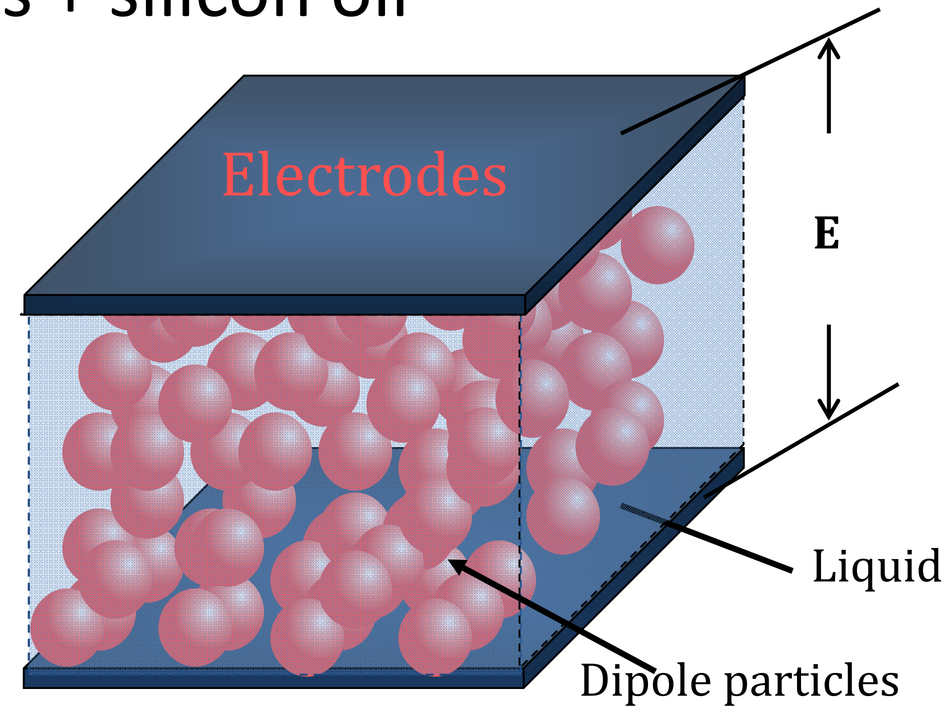
When J. K. Rowling described Harry Potter's invisibility silvery", she probably wasn't thinking specifically about silver-plated nanoparticles suspended in water. But a team of theorists believe that using such a set-up would make the first soft, tunable metamaterial – the "active ingredient" in an invisibility device.

The fluid proposed by Ji-Ping Huang of Fudan University in Shanghai, China, and colleagues, contains magnetite balls 10 nanometres in diameter, coated with a 5-nanometre-thick layer of silver, possibly with polymer chains attached to keep them from clumping

2. Experiment – Equilibrium

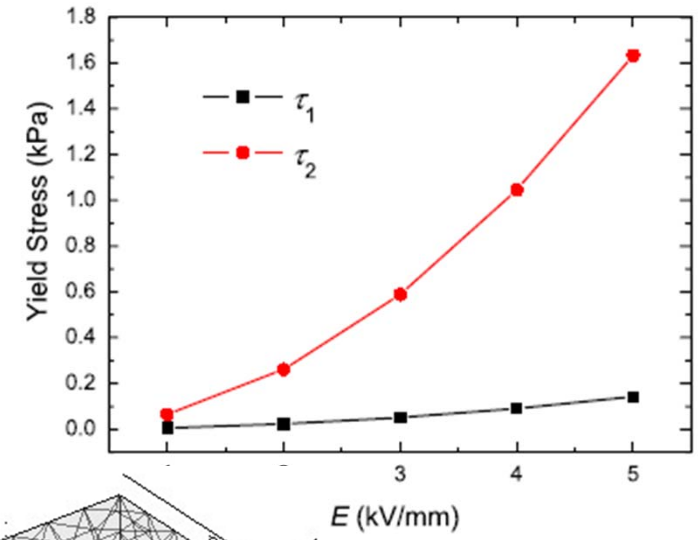
Background of ER Fluids

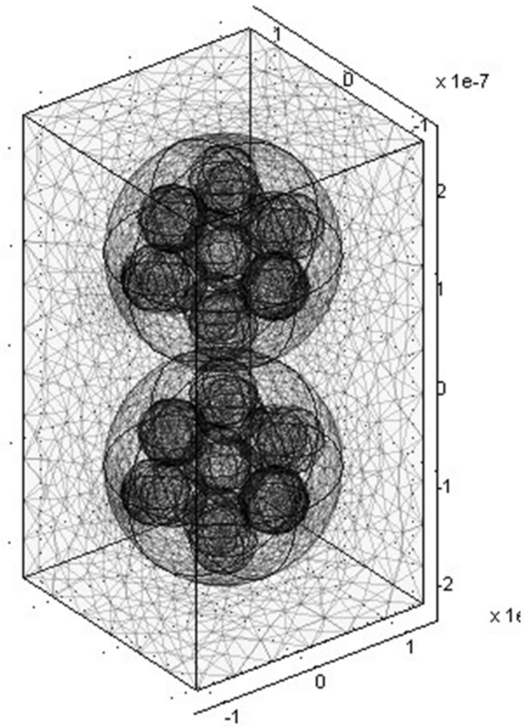
- ER (electrorheological) fluids？
  PM-ER (polar molecule dominated ER) fluids？
- ER particles + silicon oil



- Volume fraction fixed,
- Adjust parameters and re-meshing

Z.N. Fang, H.T. Xue, W. Bao, Chem. Phys. Lett. 441 (2007) 314–317.





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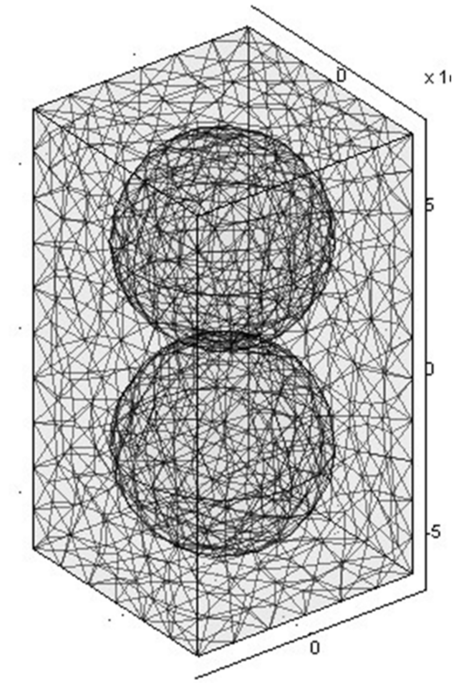
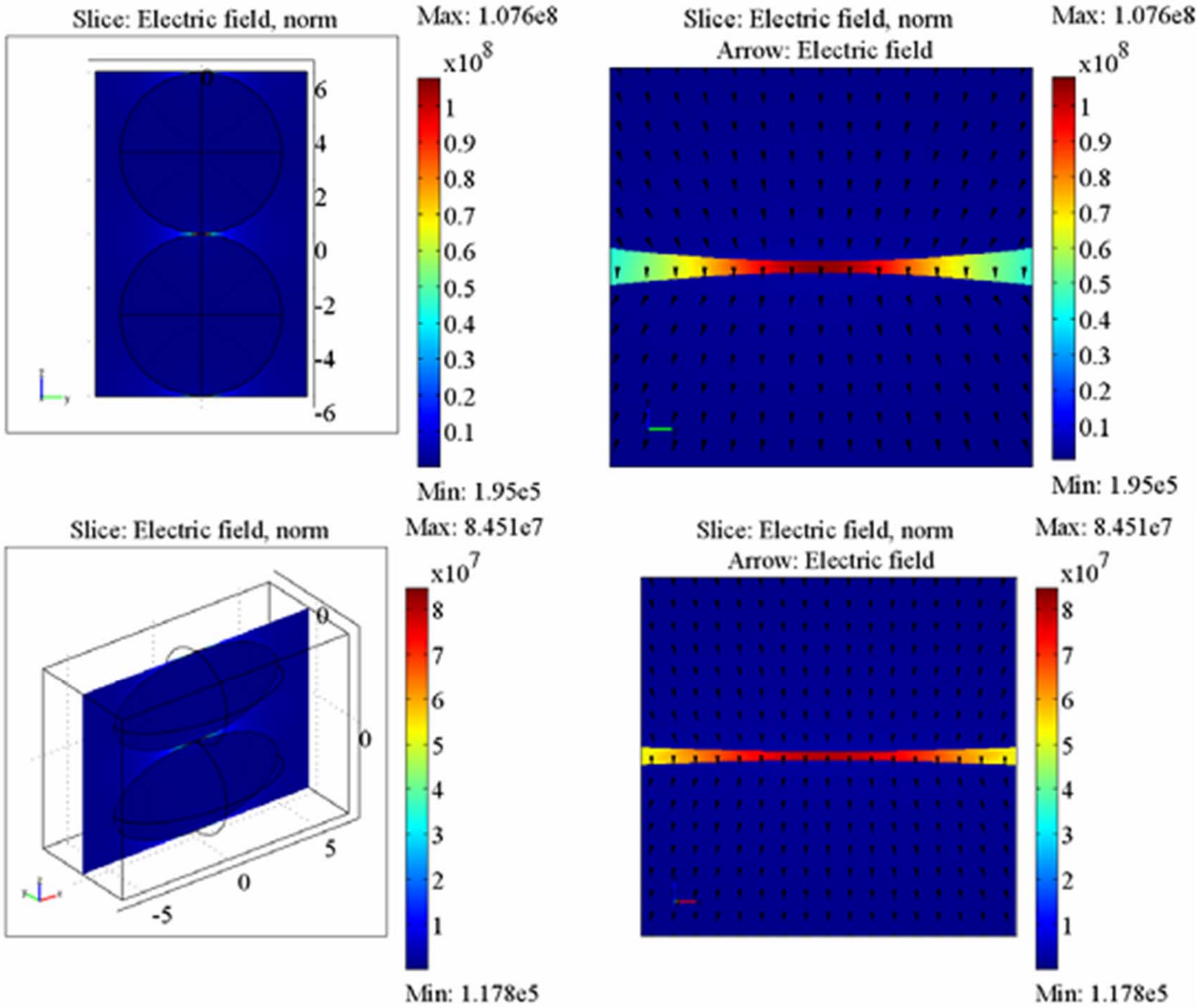


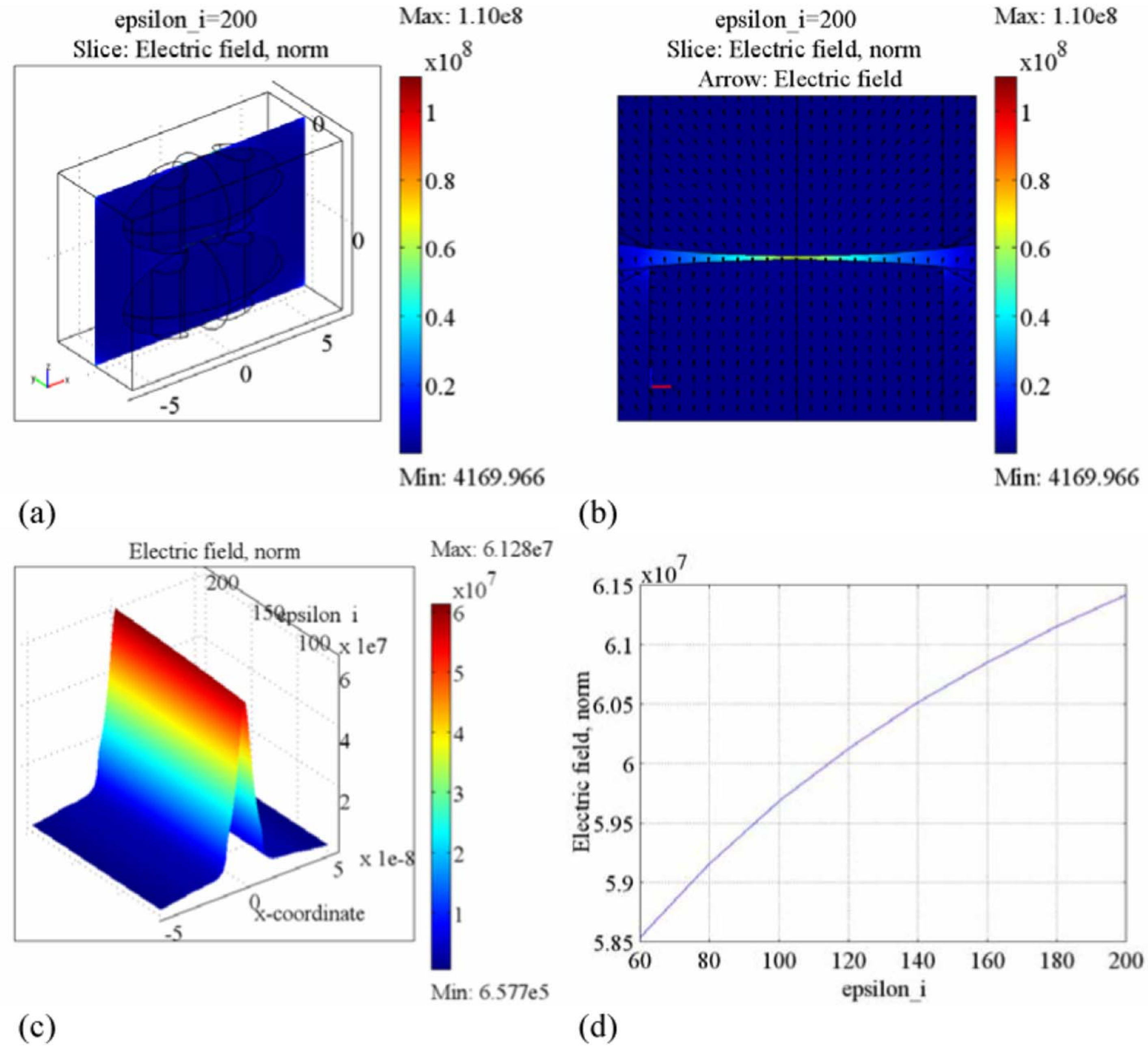
Aggregated versus well dispersed

Ratio of yield stress **1** **:** **~100**

Local electric field between two spheres



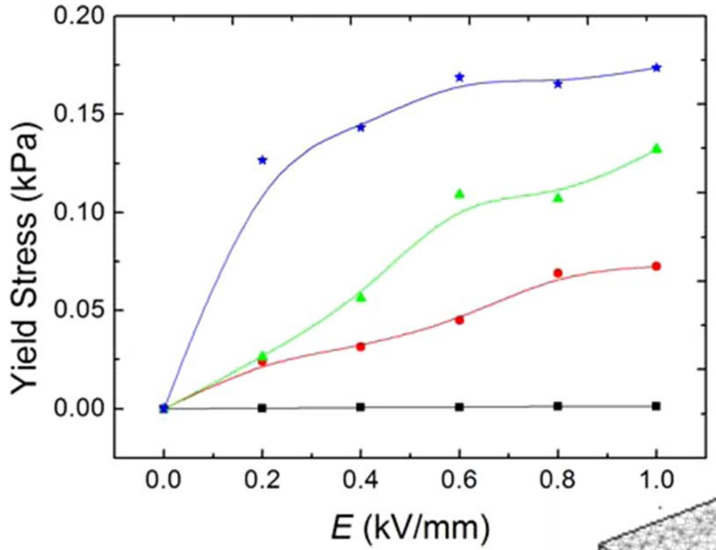
Local electric field between two ellipsoids

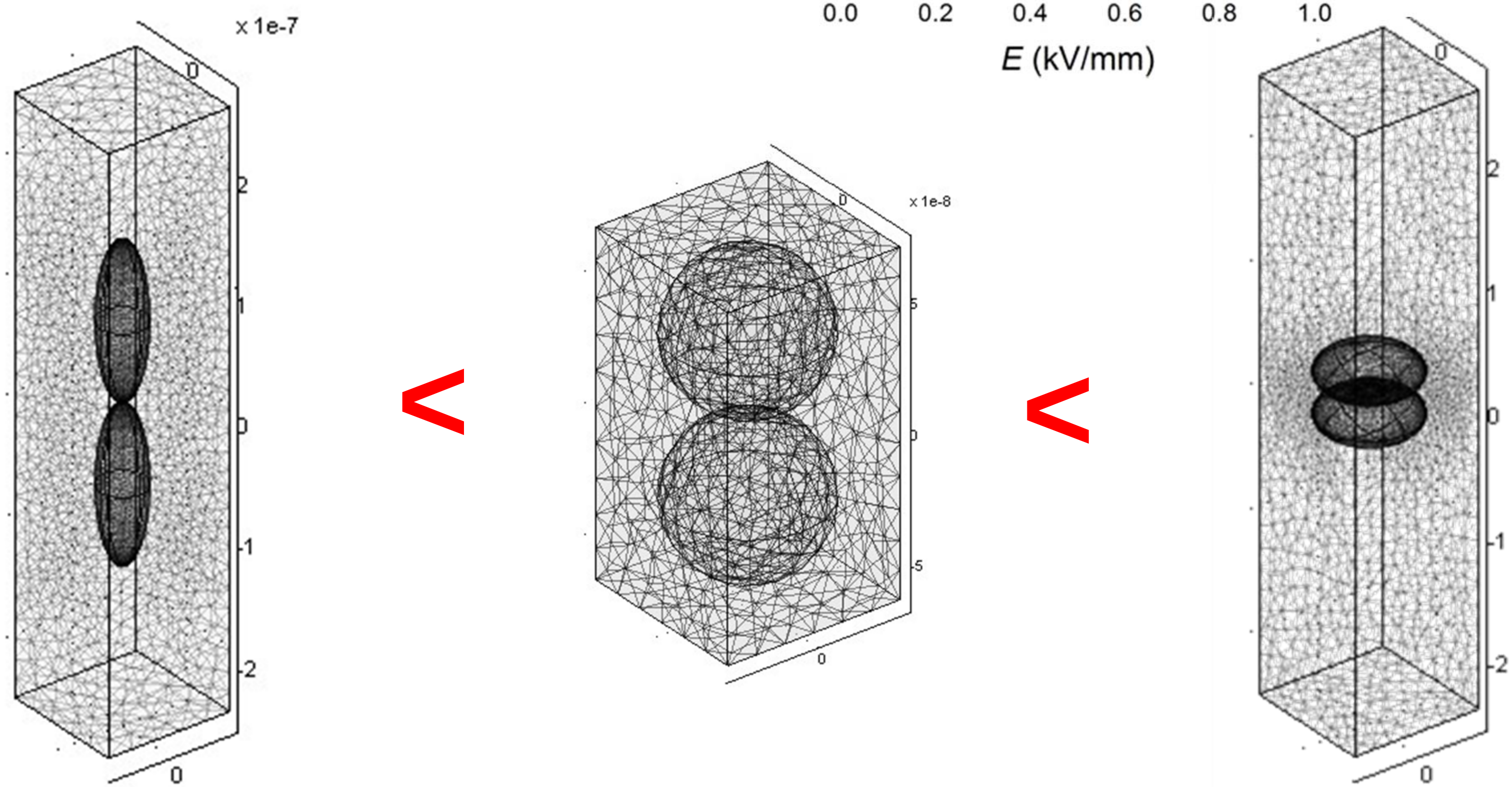


(a) (b) (c) (d)

The yield stress between two short axis chained ellipsoid particles is the largest.

Wei BAO, et al., J. Phys.- Cond. Mat. 22 (2010) 324105

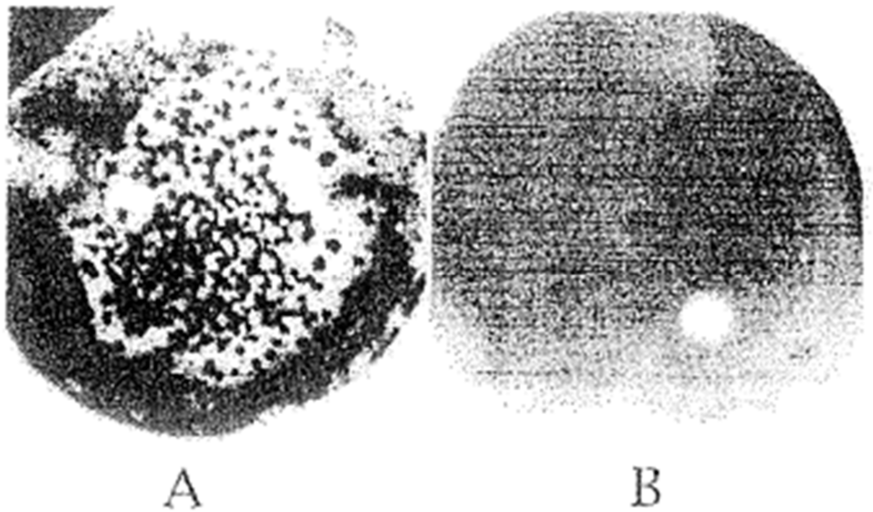




3. Experiment – Nonequilibrium

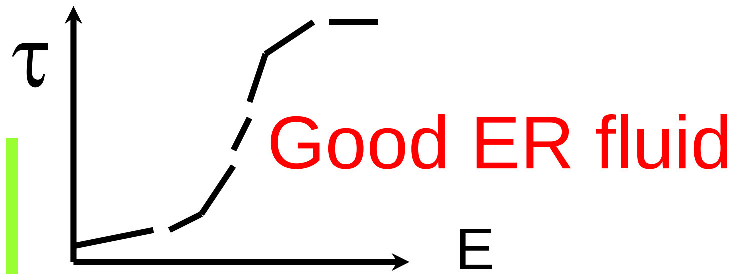
3.1 **Lamellar structures** of ER fluids under electric field and shear flow

Polystyrene ER fluid (A, B)

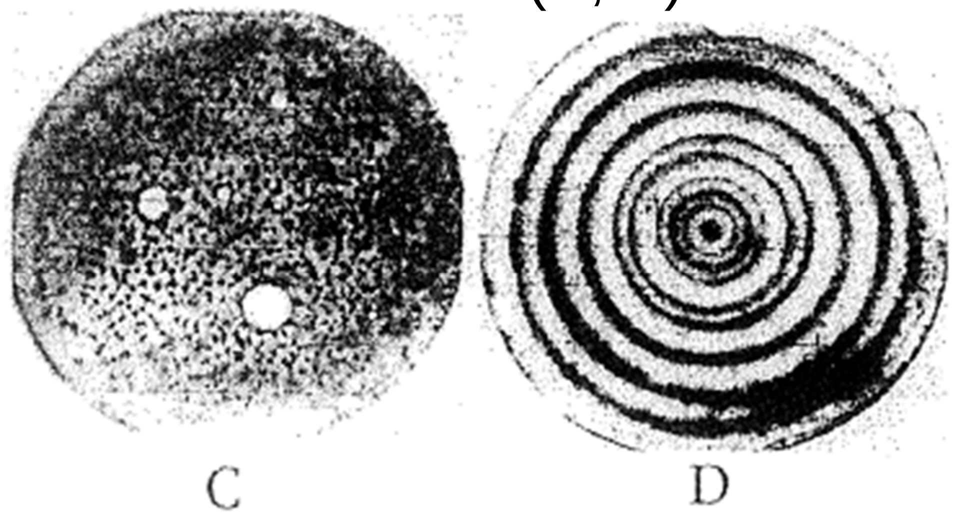


$\dot{\gamma} = 0$ $\dot{\gamma} > 0$

$E > E_c$



Sulfonated polystyrene ER fluid (C, D)

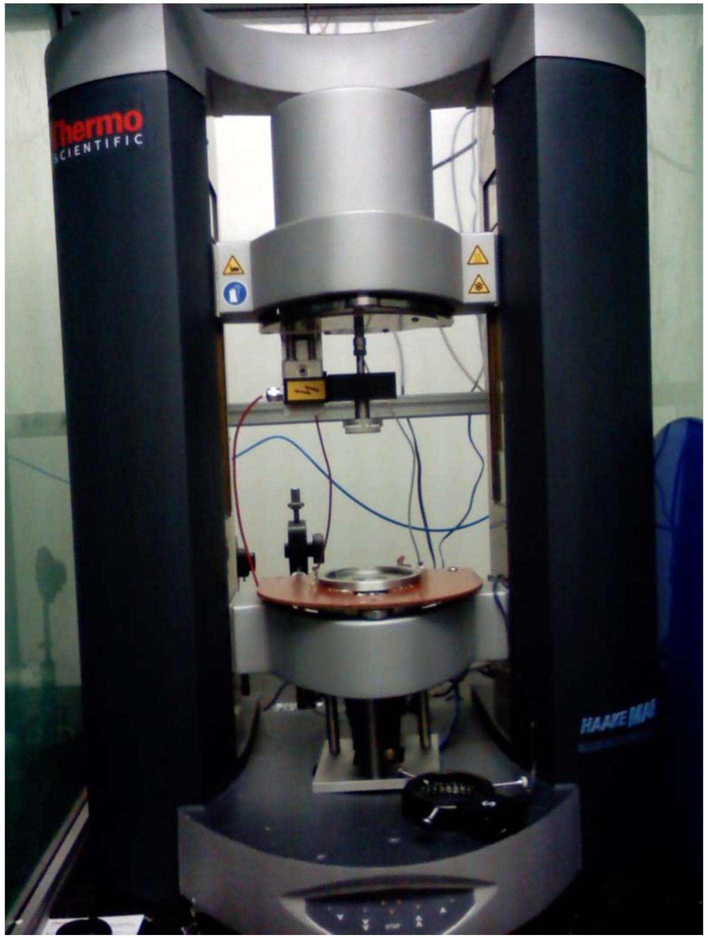


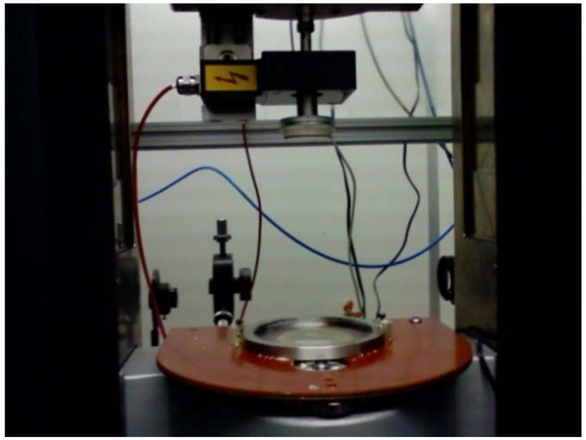
$\dot{\gamma} = 0$ $\dot{\gamma} > 0$

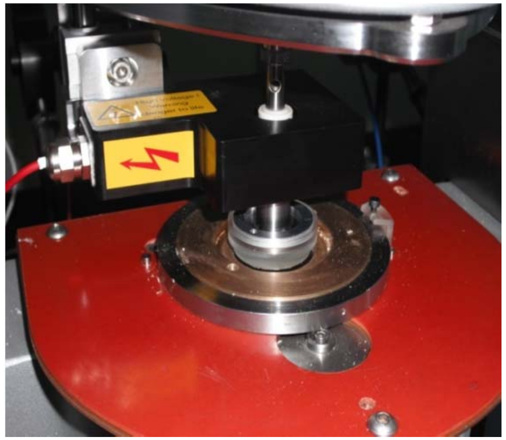
$E > E_c$

S. Henley and F. E. Filisco, Inter. J. Mod. Phys. B, 16 (2002) 2286 – 2292.

Experimental Setup



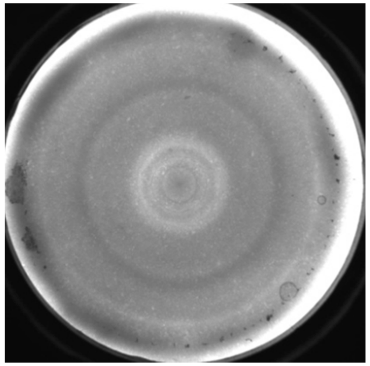




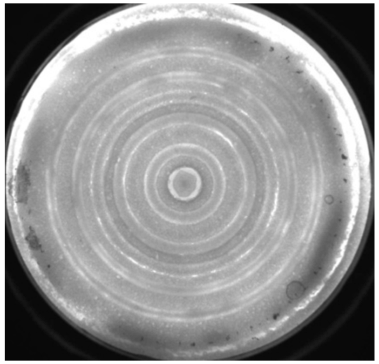
Haake Mars II rheometer → **<u>Electrorheoscope</u>**

Modified by Tan P, Liu D.K, Jia Y, Zhou L.W. et al

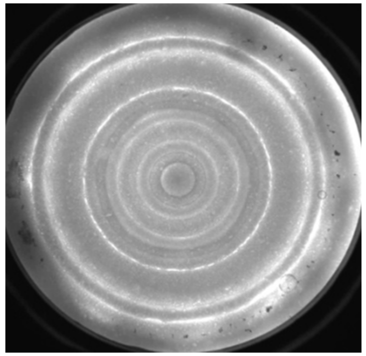
Lamellar Structures of a PM-ER Fluid under Different Electric Fields



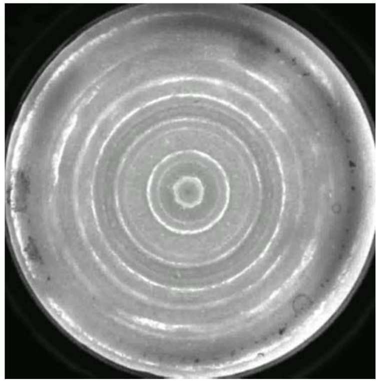
400



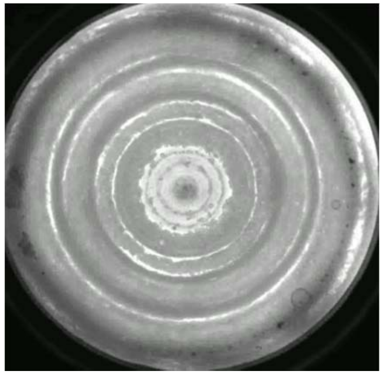
600



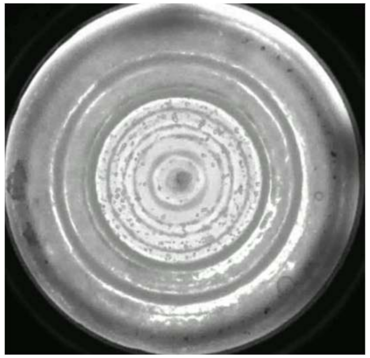
800V/mm



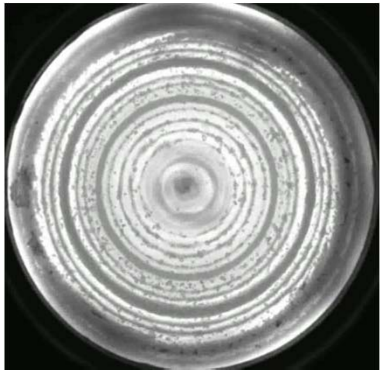
1k



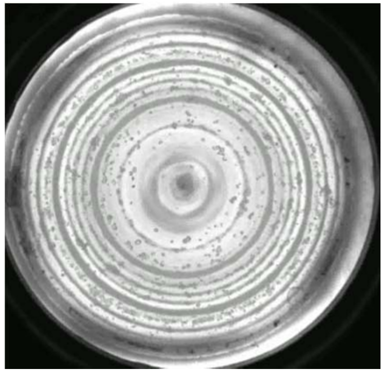
1.2k



1.4kV/mm

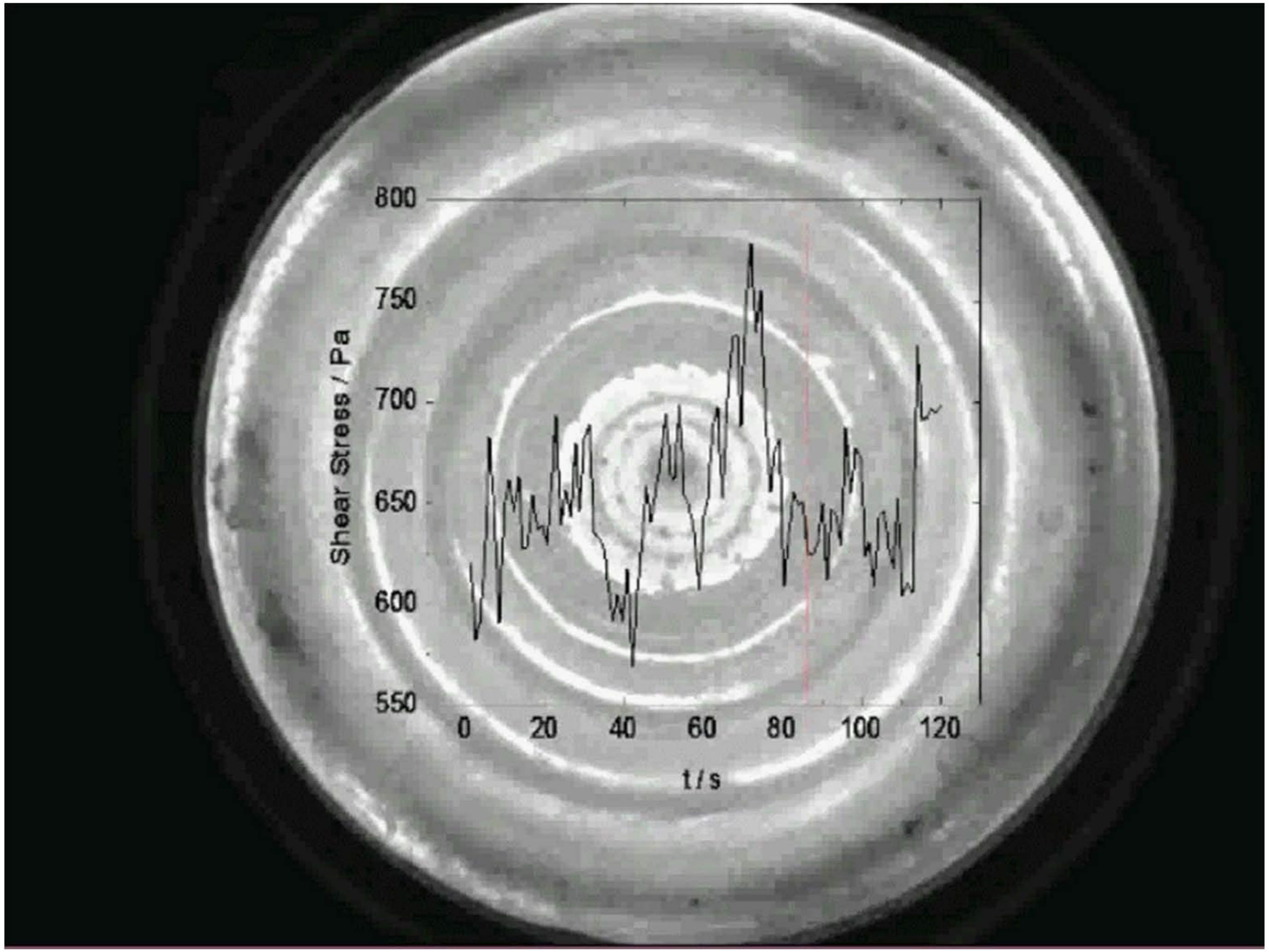


1.6k

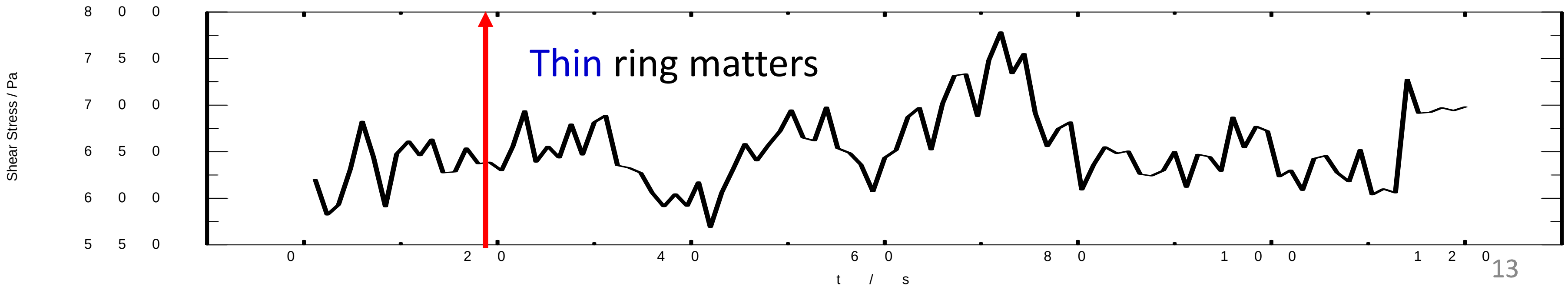


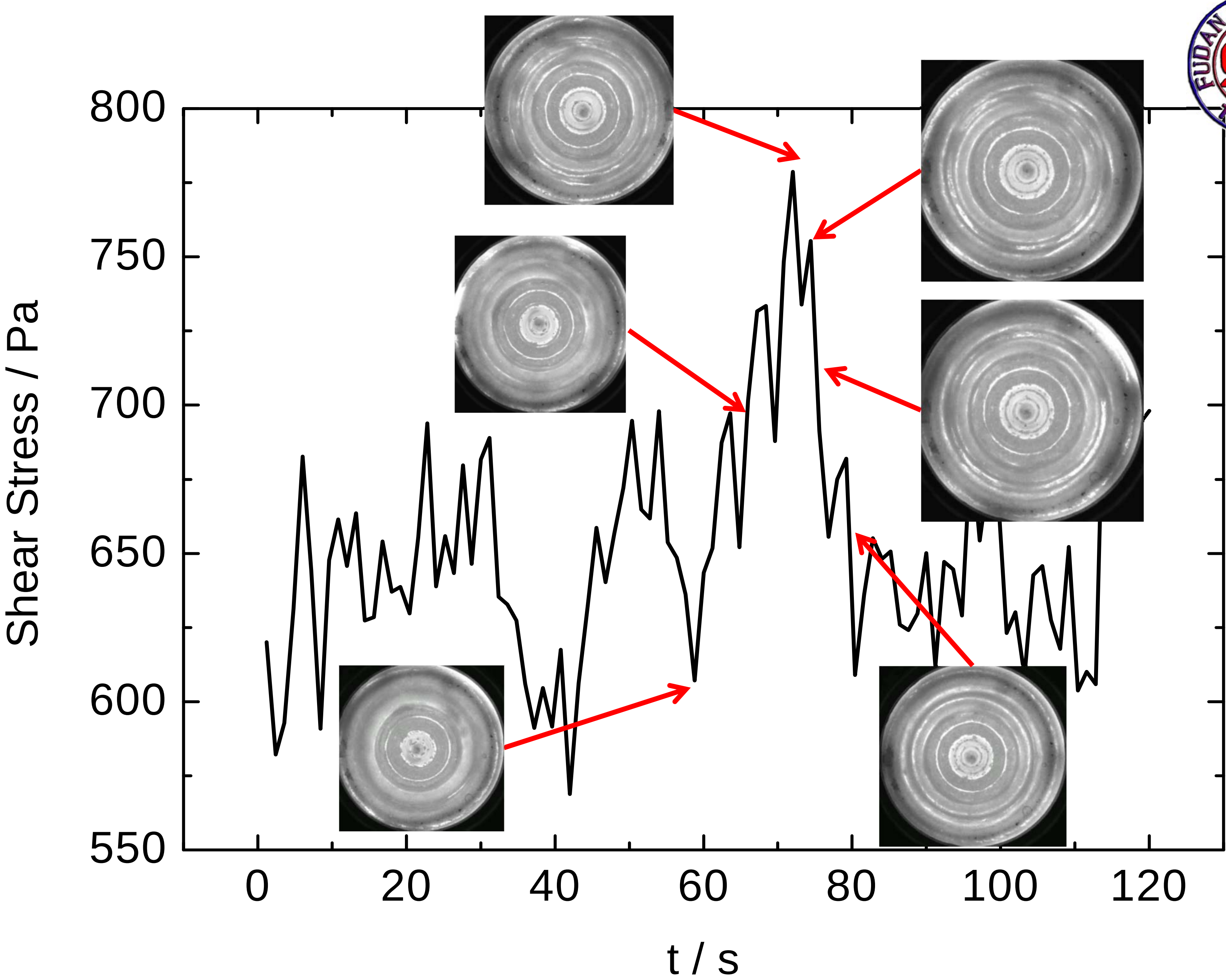
1.8k

2kV/mm

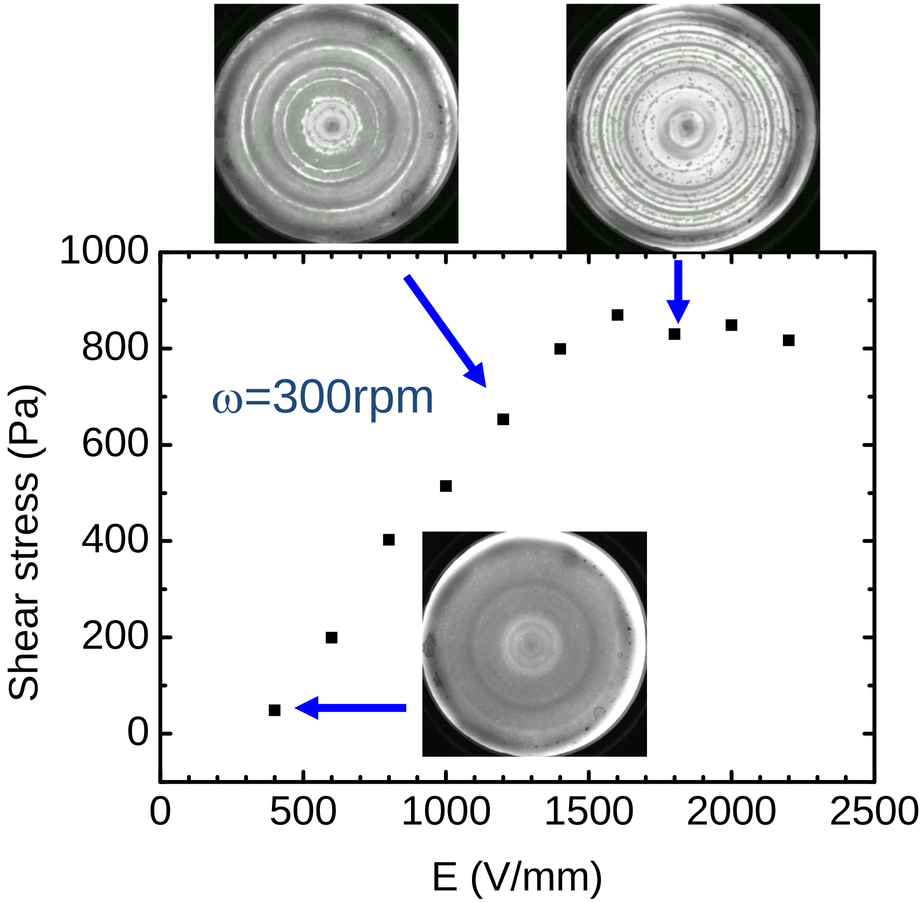


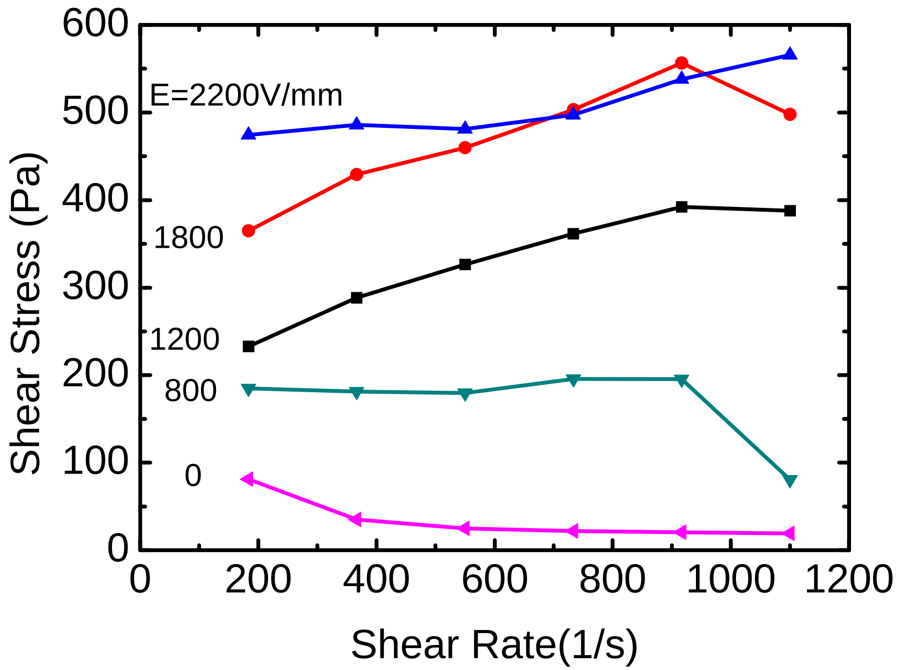
Simultaneous observation and comparison of lamellar structure and shear stress of the PM-ER fluids




Shear Stress / Pa
800
750
700
650
600
550
0
20
40
60
80
100
120
t / s

Simultaneous measurement of ER shear stress and observation of lamellar structures





3.2 **Simulation**:

Method and Theory

- Molecular dynamics (MD)
  based on Newton's second law of motion

  -- **Large amount of calculation, time-consuming**

- Two phase flow
  based on Onsager's principle with COMSOL

  -- **Easy to learn, quick calculation, powerful**

Onsager's Principle

- The Onsager's principle of minimum energy dissipation rate is about the rules governing the optimal paths of deviation and restoration to equilibrium.

$$\eta\dot{\alpha} = -\frac{\partial F(\alpha)}{\partial \alpha} + \xi(t)$$

$$A \approx \left[\frac{\eta}{2}\dot{\alpha}^2 + \frac{\partial F(\alpha)}{\partial \alpha}\dot{\alpha}\right]\Delta t$$

$$A(\vec{J}, \vec{V}_S) = \dot{F} + \Phi \quad \text{Minimum}$$

L. Onsager and S. Machlup, *Phys. Rev.* 91, 1505-1512 (1953).

L. D. Landau and E. M. Lifshitz, *Statistical Physics, 2nd Ed.,* London: Addison-Wesley Publishing Co., 1-484 (1969).

Onsager's Principle

- The modified Onsager action functional, *A*

$$A(\vec{J}, \vec{V}_S) = \dot{F} + \Phi$$

Free energy

$$F[n(\vec{x})] = \frac{1}{2}\int G_{ij}(\vec{x},\vec{y})\, p_i(\vec{x}) n(\vec{x})\, p_j(\vec{y}) n(\vec{y})\, d\vec{x} d\vec{y}$$

$$-\int \vec{E}_{ext}(\vec{x}) \cdot \vec{p}(\vec{x}) n(\vec{x})\, d\vec{x} + \frac{\varepsilon_0}{2}\int \left(\frac{a}{|\vec{x}-\vec{y}|}\right)^{12} n(\vec{x}) n(\vec{y})\, d\vec{x} d\vec{y},$$

Dissipation

$$\Phi = \int \left(\frac{1}{4}\eta_S [\partial_i (\vec{V}_S)_j + \partial_j (\vec{V}_S)_i]^2 + \frac{\gamma}{2n} J^2 + \frac{1}{2} K (\vec{V}_f - \vec{V}_s)^2 \right) d\vec{x}$$

J. W. Zhang, X. Q. Gong, C. Liu, W. J. Wen, P. Sheng, *Phys. Rev. Lett.* 101, 194503 (2008)

Onsager's Principle

Governing equations

Navier-Stokes equation for particles

$$\rho_s(\frac{\partial \vec{V}_s}{\partial t} + \vec{V}_s \cdot \nabla \vec{V}_s) = -\nabla p_s + \nabla \cdot \tau^s_{visc} + \nabla \cdot \tau_s + K(\vec{V}_f - \vec{V}_s)$$

Navier-Stokes equation for oil

$$\rho_f(\frac{\partial \vec{V}_f}{\partial t} + \vec{V}_f \cdot \nabla \vec{V}_f) = -\nabla p_f + \nabla \cdot \tau^f_{visc} + K(\vec{V}_s - \vec{V}_f)$$

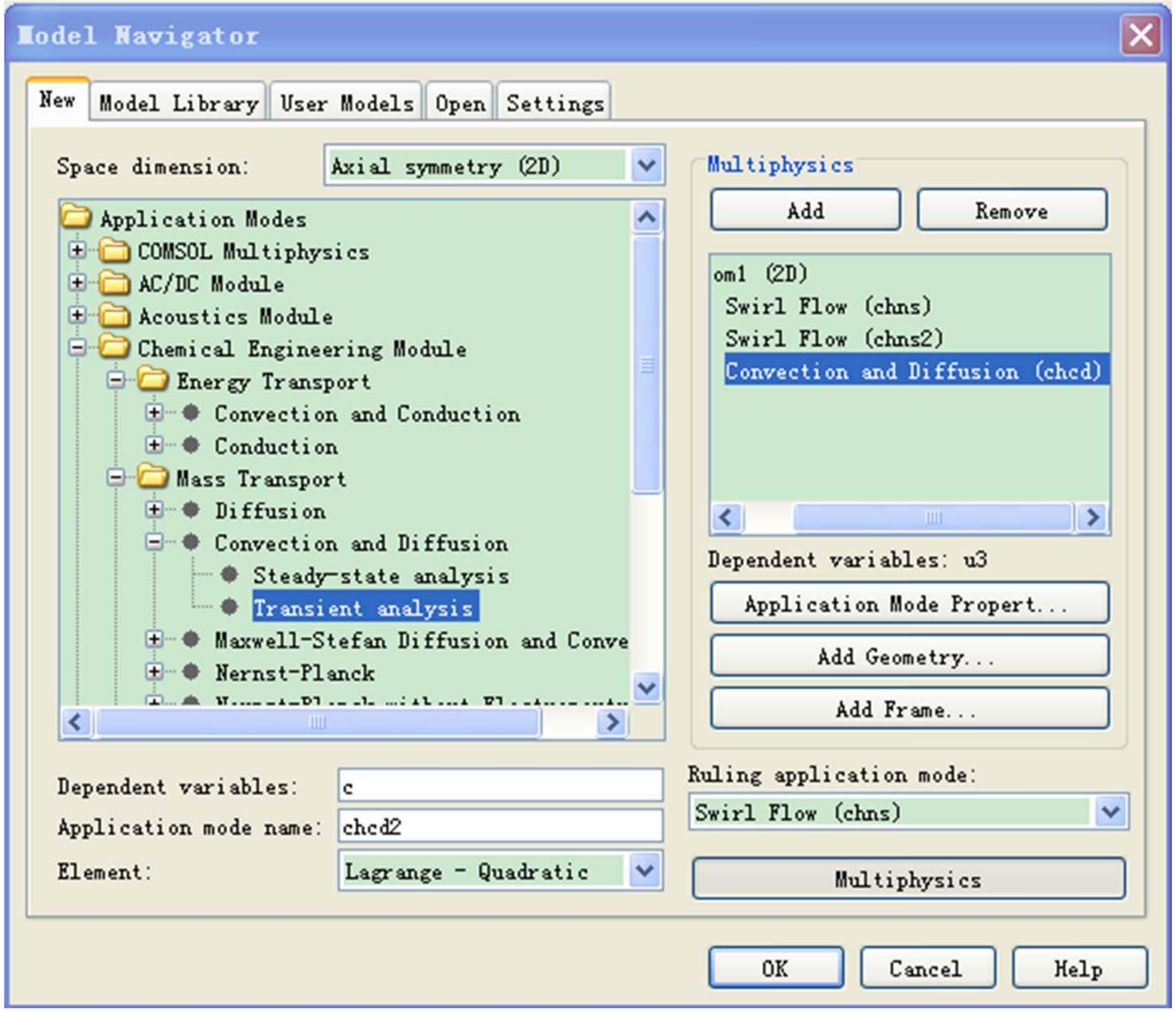
Continuity equation

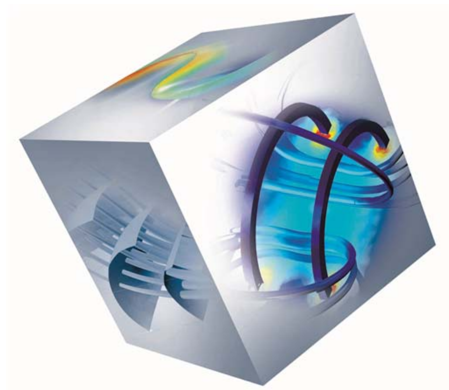
$$\dot{n} + \vec{\nabla} \cdot \vec{J} = \partial_t n + V_s \cdot \vec{\nabla} n + \vec{\nabla} \cdot \vec{J} = 0$$

J. W. Zhang, X. Q. Gong, C. Liu, W. J. Wen, P. Sheng, *Phys. Rev. Lett.* 101, 194503 (2008)

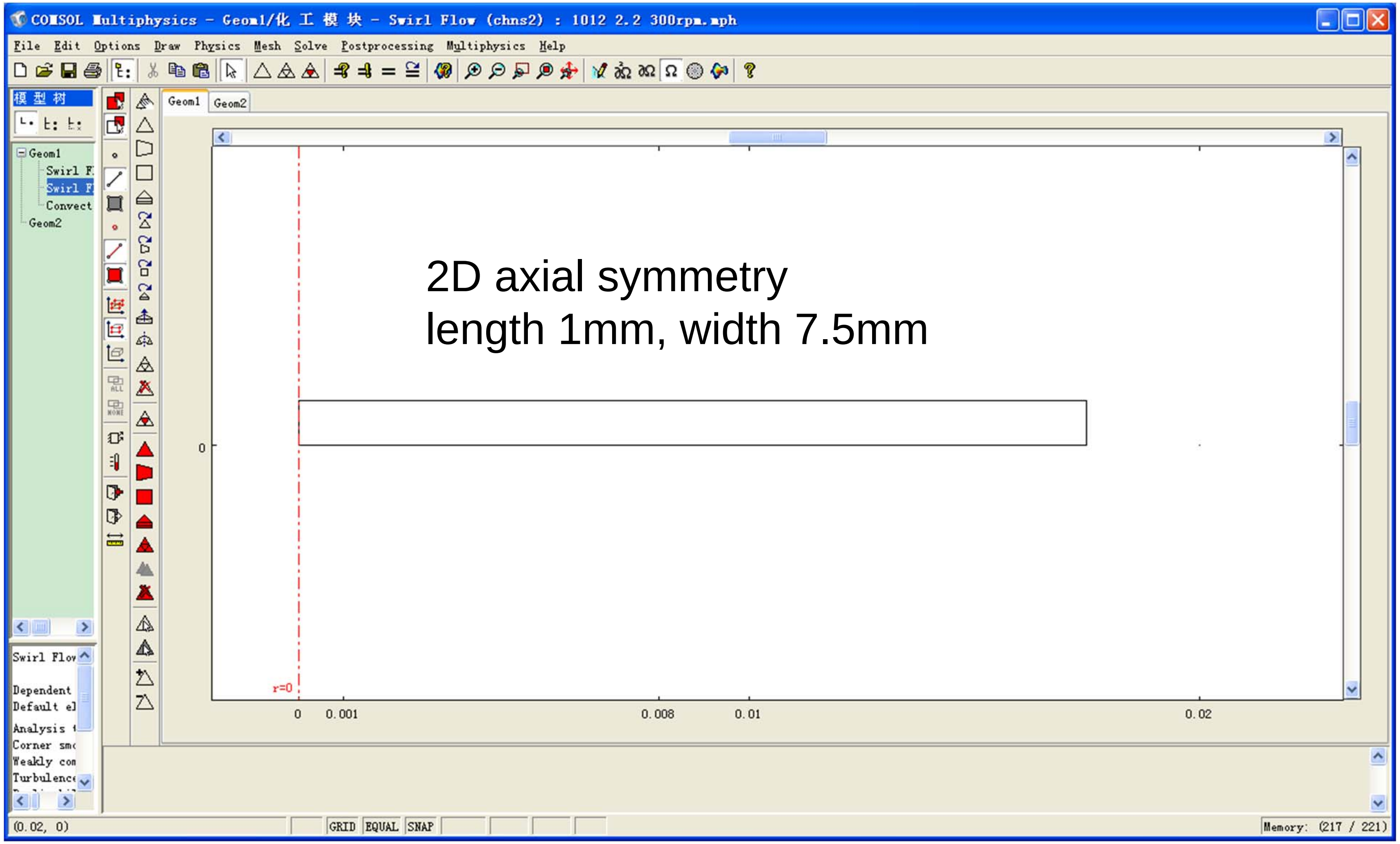
COMSOL Simulation

a. Model Establishment





b. Geometry


COMSOL Multiphysics - Geom1/化 工 模 块 - Swirl Flow (chns2) : 1012 2.2 300rpm.mph
File Edit Options Draw Physics Mesh Solve Postprocessing Multiphysics Help
Geom1
Geom2
2D axial symmetry
length 1mm, width 7.5mm
r=0
0
0.001
0.008
0.01
0.02
GRID EQUAL SNAP
Memory: (217 / 221)

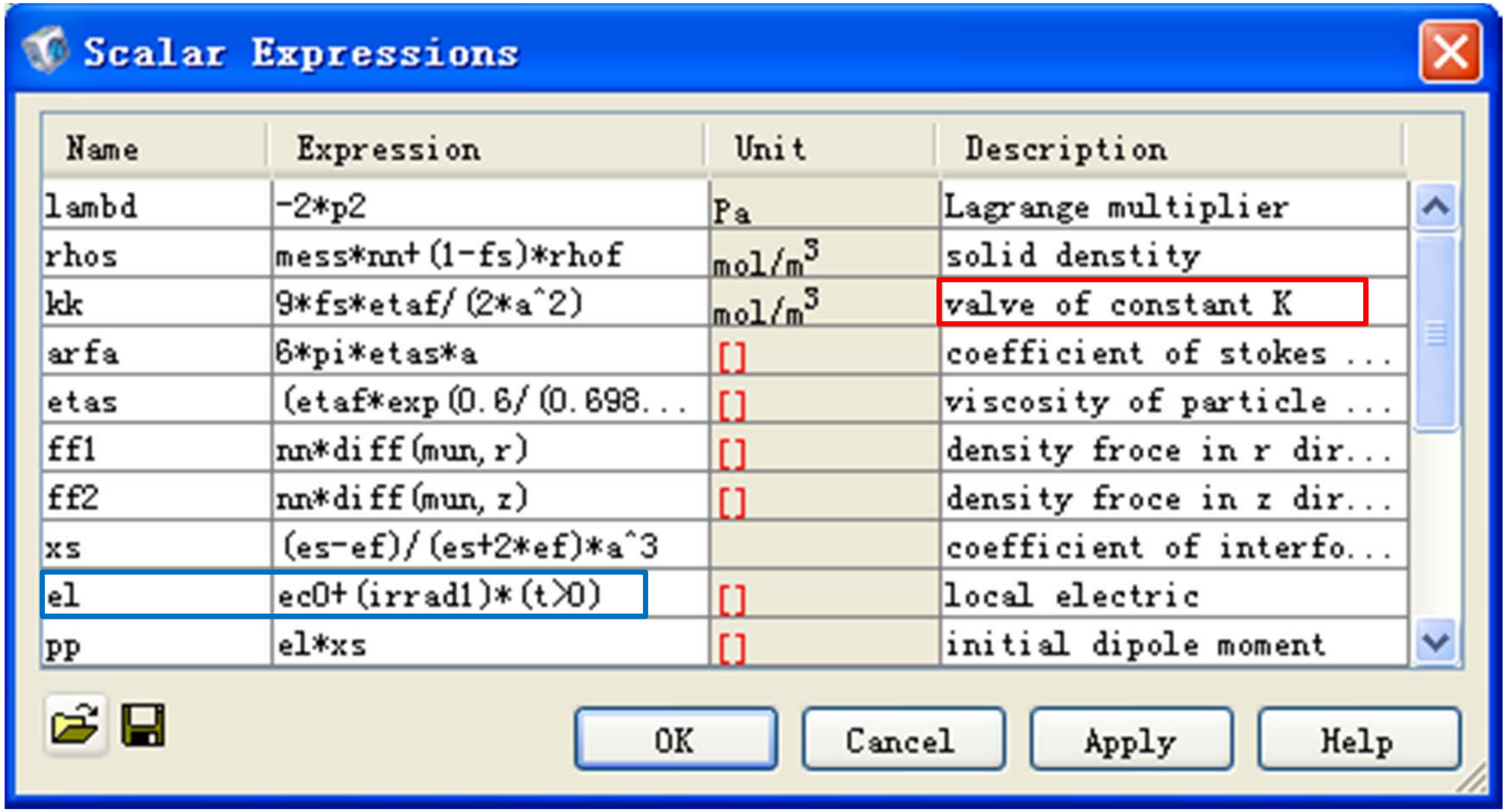
c. Parameters

Constants

Name	Expression	Value	Description
omega	10*pi[rad/s]	31.41592	Angular velocity
rhof	960	960	density of fluid
etaf	0.01	0.01	viscosity of fluid
ef	2	2	dielectric constant of fluid
a	5e-7	5e-7	radius of particle
mess	1.2e-12	1.2e-12	mess of one particle
es	40	40	dielectric constant of particle
ec0	1000000*0.4	4e5	E filed
r0	0.0000011	1.1e-6	smallest distandence between two particles
ebsilon0	6.6e-1	0.66	energy constant of repulsive potential
tstep	0.000000001	1e-9	time step
naa	6.022*10^23	6.02...	Avogadro's constant

OK Cancel Apply Help

d. Expressions

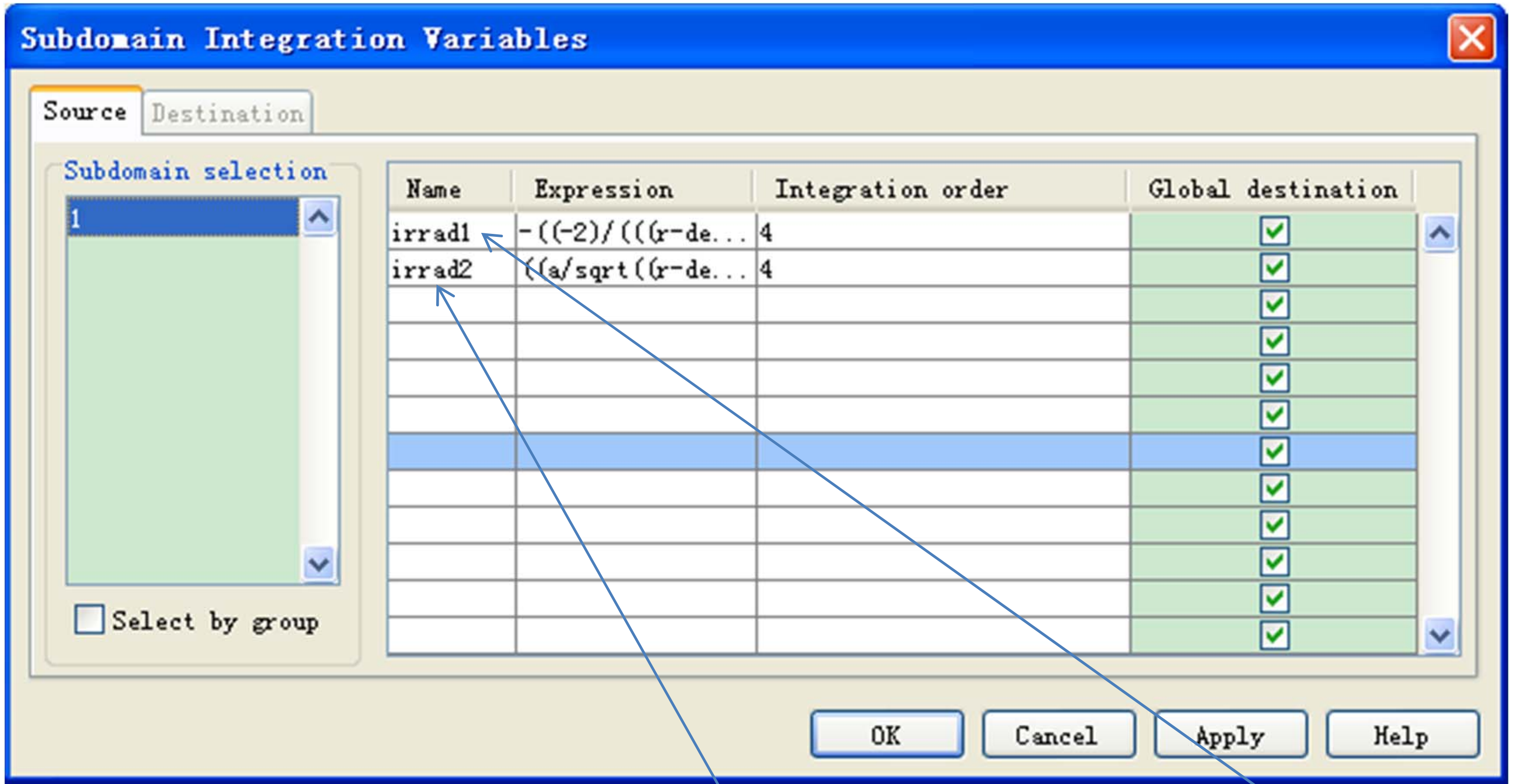


Name	Expression	Unit	Description
lambd	-2*p2	Pa	Lagrange multiplier
rhos	mess*nn+(1-fs)*rhof	mol/m^3	solid denstity
kk	9*fs*etaf/(2*a^2)	mol/m^3	valve of constant K
arfa	6*pi*etas*a	[]	coefficient of stokes ...
etas	(etaf*exp(0.6/(0.698...	[]	viscosity of particle ...
ff1	nn*diff(mun,r)	[]	density froce in r dir...
ff2	nn*diff(mun,z)	[]	density froce in z dir...
xs	(es-ef)/(es+2*ef)*a^3		coefficient of interfo...
el	ec0+(irrad1)*(t>0)	[]	local electric
pp	el*xs	[]	initial dipole moment

el: Local electric field, **ff1&ff2**: Conservative force,

kk: Stokes drag force density $K = 9 f_s \eta_f / 2a^2$

e. Integration Coupling Variables



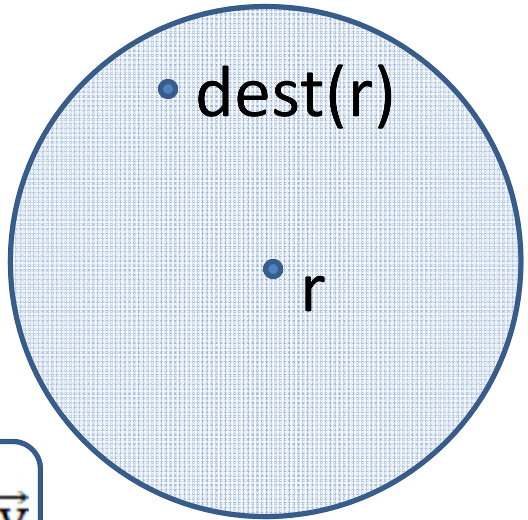
Local electric field $[\vec{E}_l(\vec{x})]_i = [\vec{E}_{ext}(\vec{x})]_i + \int G_{ij}(\vec{x},\vec{y})\, p_j(\vec{y})\, n(\vec{y})\, d\vec{y}$

Repulsive potential $\varepsilon_0 \int \left(\frac{a}{|\vec{x}-\vec{y}|} \right)^{12} n(\vec{y})\, d\vec{y}$

dest() operator

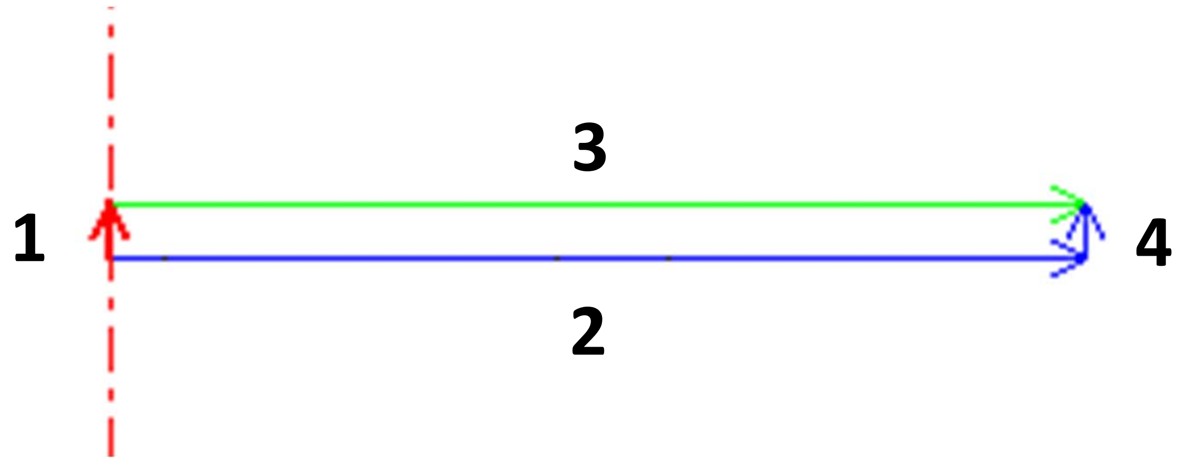
- Irrad1=-((-2)/((((r-dest(r))^2+(z-dest(z))^2)^3)*dest(nn)*dest(pp2))*((sqrt((r-dest(r))^2+(z-dest(z))^2)<=10*a)*(sqrt((r-dest(r))^2+(z-dest(z))^2)>=2.1*a))

dest() is a operator to create convolution integral



$$[\vec{E}_l(\vec{x})]_i = [\vec{E}_{ext}(\vec{x})]_i + \int G_{ij}(\vec{x},\vec{y})\, p_j(\vec{y}) n(\vec{y}) d\vec{y}$$

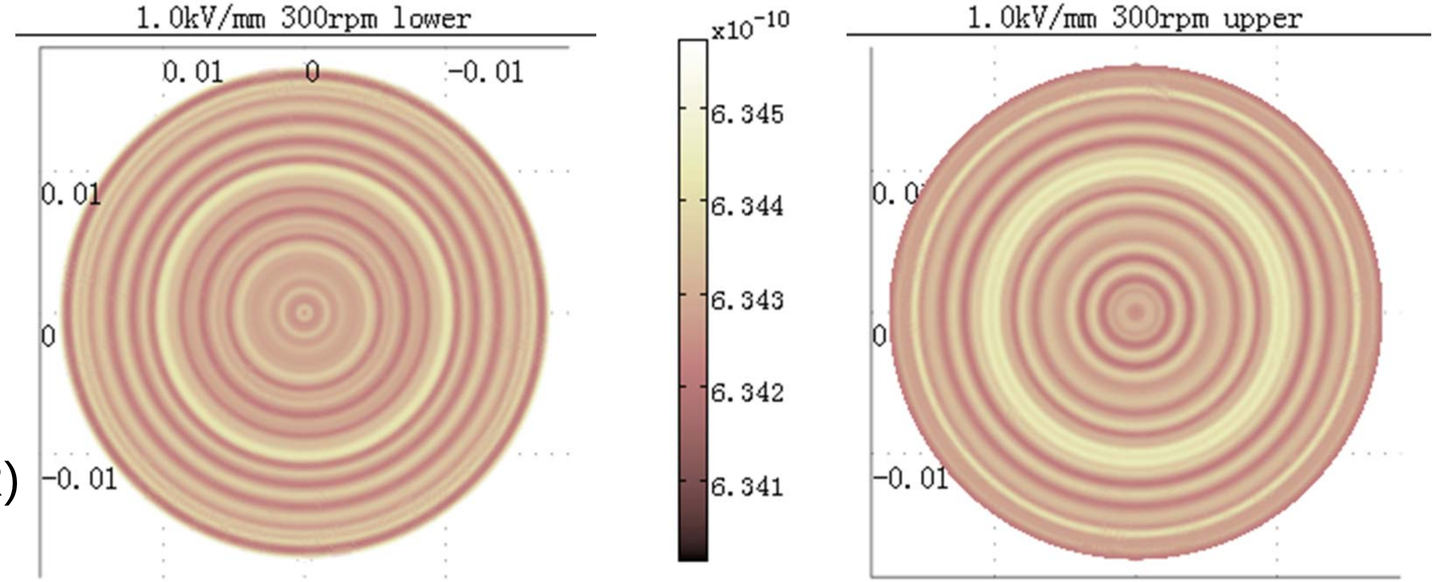
e. Boundary Conditions



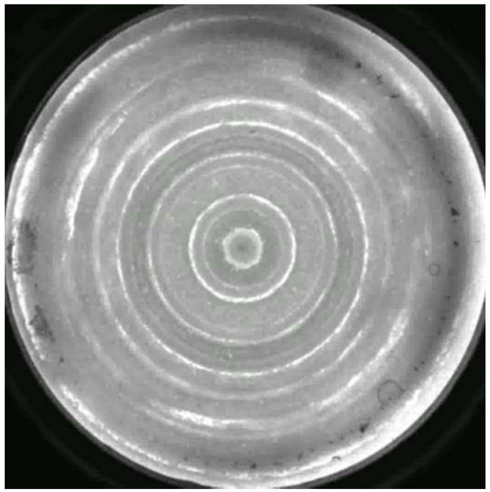
	Oil phase	Particle phase	Concentration
1	Axial symmetry	Axial symmetry	Symmetry / Insulation
2	Logarithmic wall function	Wall / No slip	Symmetry / Insulation
3	Sliding wall / omega*r	Sliding wall / omega*r	Symmetry / Insulation
4	Logarithmic wall function	Wall / No slip	Symmetry / Insulation

f. Results

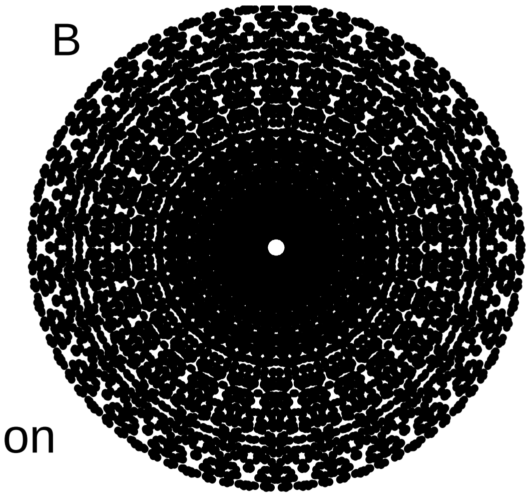
COMSOL pattern simulations of upper (L) and lower (R) electrodes



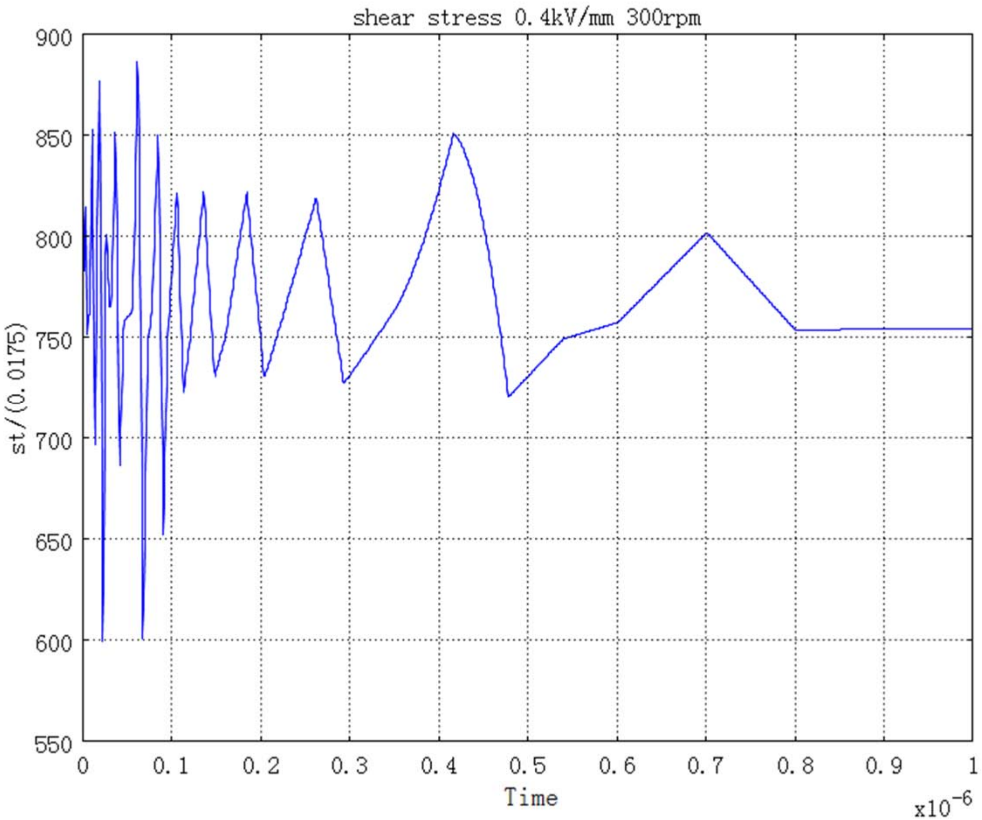
Experimental observation



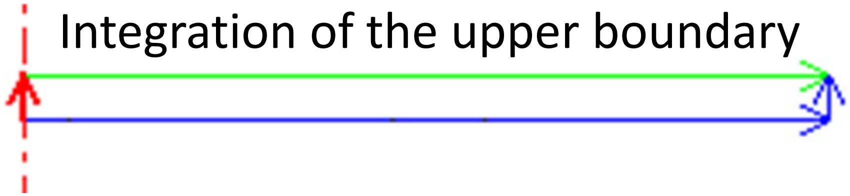
MD simulation

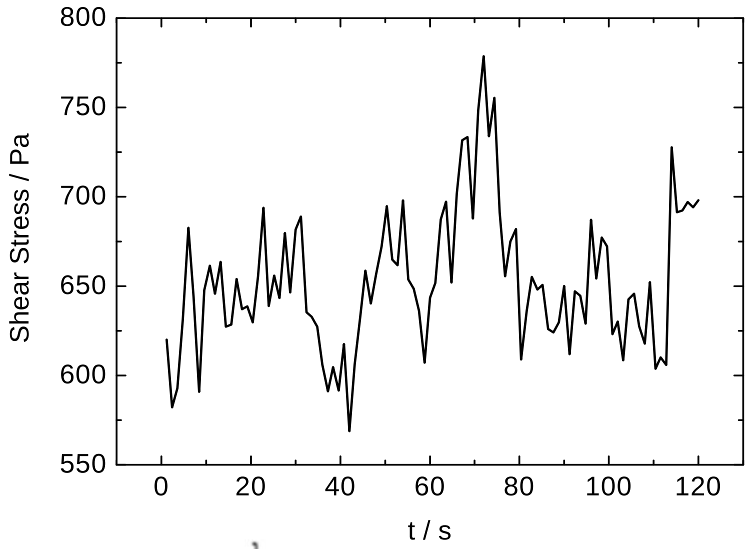


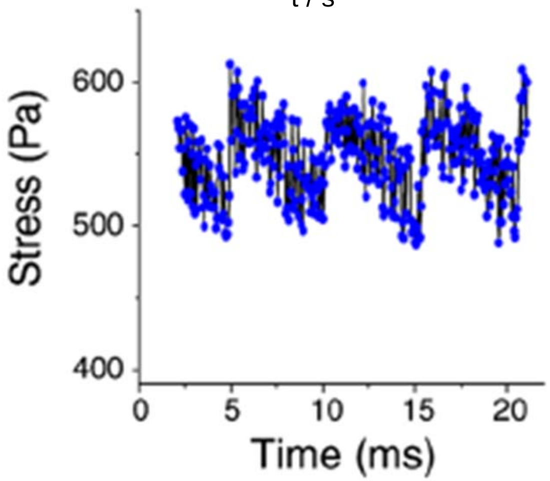
Shear Stress



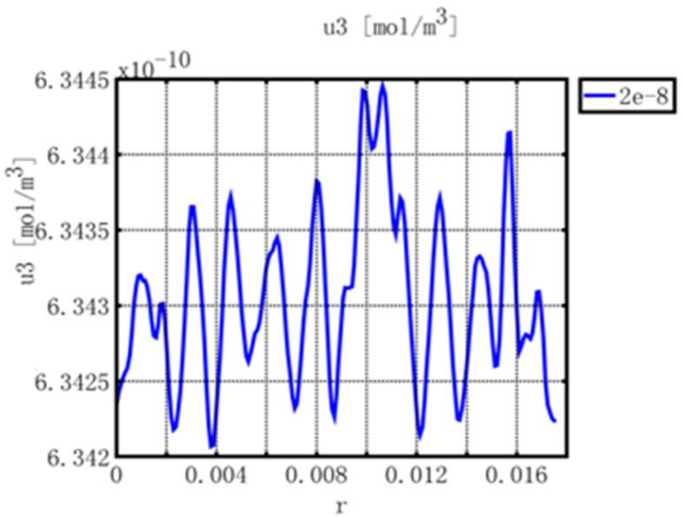
Integration of the upper boundary

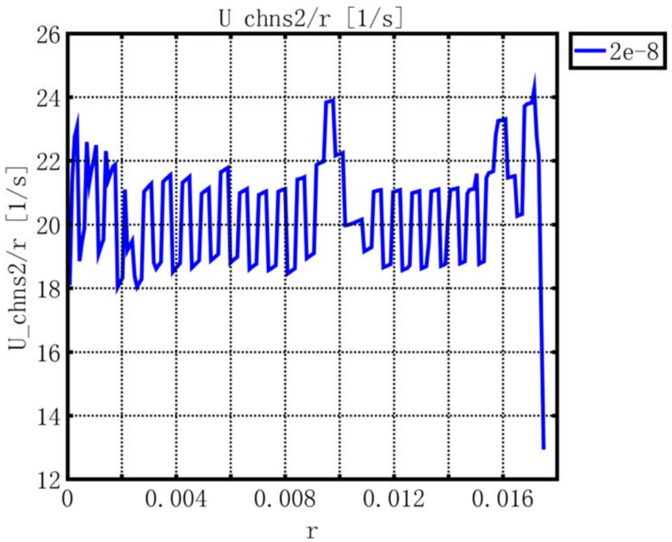


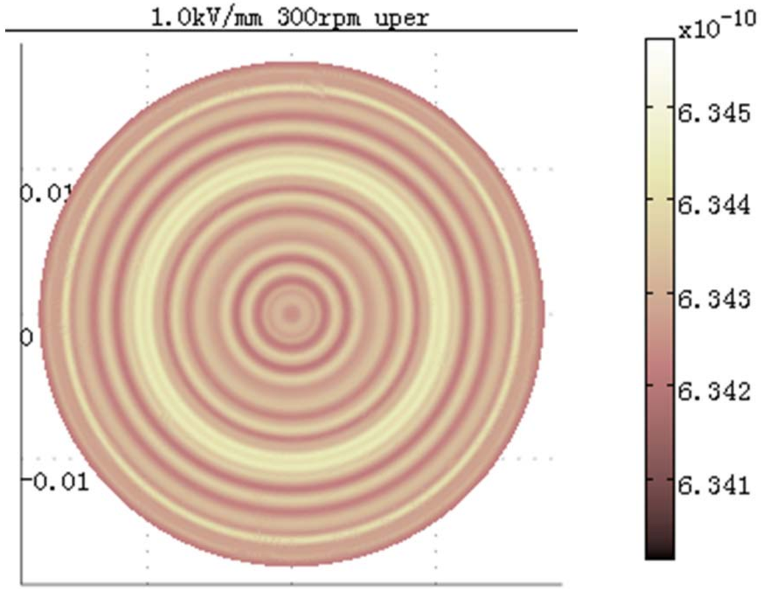




Conclusion：
Static and Dynamic Rings







The angular velocity changes along the radius. Regions with high velocity and low velocity exist in the subdomain.

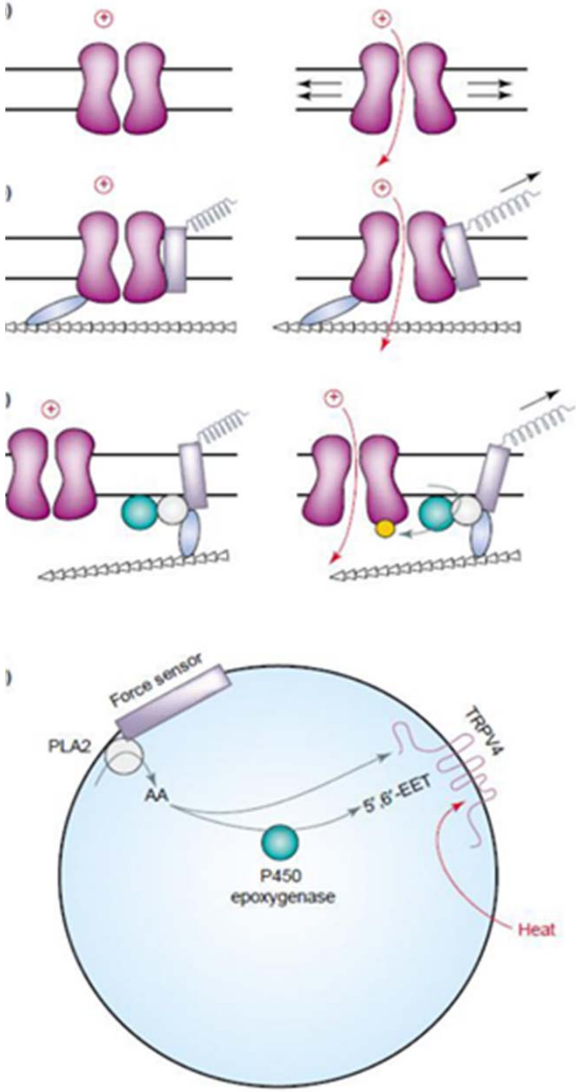
It is the dynamic ring that have the maximum concentration and velocity.

4. Future Work

- Pattern and force with different slip lengths
- Quantitative relations between shear stress and lamellar structures
- Relation of patterns and shear stress under AC field
- Different temperature effect

-- All students in soft matter group must study **COMSOL Multiphysics**

Expending to biophysics and granules



We should spread COMSOL to China's western region such as Xinjiang and Gansu

TRPchannels in mechanosensation,Current Opinion in Neurobiology 2005,15:350-357

Thank you very much

State Key Laboratory of Surface Physics
and Physics Department
Fudan University