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


Hard $\rightarrow$ Soft metamaterials
Single frequency $\rightarrow$ Broad band frequencies
Optic Invisibility $\rightarrow$ Acoustic Invisibility

Wavelength 758nm 3D

LIQUID LIGHT BENDER PROPOSED

Tiny nanoparticles dispersed in fluid may hide objects

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

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...
Background of ER Fluids

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

2. Experiment – Equilibrium

Electrodes

Liquid

Dipole particles

\[ E \]
• Volume fraction fixed,
• Adjust parameters and re-meshing


Aggregated versus well dispersed
Ratio of yield stress $1$ : $\sim 100$
Local electric field between two spheres
Local electric field between two ellipsoids
The yield stress between two short axis chained ellipsoid particles is the largest.

3. Experiment – Nonequilibrium

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

Bad ER fluid
Polystyrene ER fluid (A, B)
\[ \dot{\gamma} = 0 \]
\[ E > E_c \]
\[ \dot{\gamma} > 0 \]

Good ER fluid
Sulfonated polystyrene ER fluid (C, D)
\[ \dot{\gamma} = 0 \]
\[ E > E_c \]
\[ \dot{\gamma} > 0 \]

Experimental Setup

Haake Mars II rheometer → Electrorheoscope

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

- 400V/mm: 1k
- 600V/mm: 1.2k
- 800V/mm: 1.4kV/mm
- 1kV/mm: 1.6k
- 1.2kV/mm: 1.8k
- 2kV/mm:
Simultaneous observation and comparison of lamellar structure and shear stress of the PM-ER fluids
Simultaneous measurement of ER shear stress and observation of lamellar structures.

\[ \omega = 300 \text{rpm} \]

Shear stress (Pa) vs. E (V/mm) graph.

Shear stress (Pa) vs. Shear Rate (1/s) graph with different curves for different electric fields (E).

Electric field (E) values: 2200 V/mm.
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
• The Onsager’s principle of minimum energy dissipation rate is about the rules governing the optimal paths of deviation and restoration to equilibrium.

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

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

\[ A (\vec{J}, \vec{V}_S) = \vec{F} + \Phi \] **Minimum**

Onsager’s Principle

- The modified Onsager action functional, $A$

\[
A (\vec{J}, \vec{V}_s) = \dot{F} + \Phi
\]

Free energy

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

\[
- \int \vec{E}_{ext}(\vec{x}) \cdot \vec{p}(\vec{x}) n(\vec{x}) d\vec{x} + \frac{\epsilon_0}{2} \int \left( \frac{a}{|\vec{x} - \vec{y}|} \right)^{12} n(\vec{x}) n(\vec{y}) d\vec{x} d\vec{y},
\]

Dissipation

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

Onsager’s Principle

Navier-Stokes equation for particles
\[ \rho_s \left( \frac{\partial \vec{V}_s}{\partial t} + \vec{V}_s \cdot \nabla \vec{V}_s \right) = -\nabla p_s + \nabla \cdot \tau^s_{\text{visc}} + \nabla \cdot \tau_s + K(\vec{V}_f - \vec{V}_s) \]

Navier-Stokes equation for oil
\[ \rho_f \left( \frac{\partial \vec{V}_f}{\partial t} + \vec{V}_f \cdot \nabla \vec{V}_f \right) = -\nabla p_f + \nabla \cdot \tau^f_{\text{visc}} + K(\vec{V}_s - \vec{V}_f) \]

Continuity equation
\[ \dot{n} + \nabla \cdot \vec{J} = \partial_t n + V_s \cdot \nabla n + \nabla \cdot \vec{J} = 0 \]

COMSOL Simulation

a. Model Establishment
b. Geometry

2D axial symmetry
length 1mm, width 7.5mm
c. Parameters

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<th>Expression</th>
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<th>Description</th>
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<td>6.022*10^23</td>
<td>6.02...</td>
<td>Avogadro’s constant</td>
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d. Expressions

**el**: Local electric field, **ff1 & ff2**: Conservative force,
**kk**: Stokes drag force density

\[ K = \frac{9 f_s \eta_f}{2 a^2} \]
e. Integration Coupling Variables

Local electric field

\[ [E_1(x)]_i = [E_{\text{ext}}(x)]_i + \int G_{ij}(\vec{x}, \vec{y}) p_j(\vec{y}) n(\vec{y}) d\vec{y} \]

Repulsive potential

\[ \varepsilon_0 \left( \frac{a}{|x - y|} \right)^{12} n(\vec{y}) d\vec{y} \]
dest() operator

- Irrad1 = \(-((-2)/(((r - \text{dest}(r))^2 + (z - \text{dest}(z))^2)^3) \times \text{dest(nn)} \times \text{dest(pp2)}) \times ((\sqrt{(r - \text{dest}(r))^2 + (z - \text{dest}(z))^2} \leq 10a) \times (\sqrt{(r - \text{dest}(r))^2 + (z - \text{dest}(z))^2} \geq 2.1a))\)

dest() is a operator to create convolution integral

\[
\left[ E_1(\vec{x}) \right]_i = \left[ E_{\text{ext}}(\vec{x}) \right]_i + \int G_{ij}(\vec{x}, \vec{y}) p_j(\vec{y}) n(\vec{y}) d\vec{y}
\]
e. Boundary Conditions

<table>
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<tr>
<th>Oil phase</th>
<th>Particle phase</th>
<th>Concentration</th>
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<td>Axial symmetry</td>
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</tr>
<tr>
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<td>Wall / No slip</td>
<td>Symmetry / Insulation</td>
</tr>
<tr>
<td>Sliding wall / omega*r</td>
<td>Sliding wall / omega*r</td>
<td>Symmetry / Insulation</td>
</tr>
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<td>Logarithmic wall function</td>
<td>Wall / No slip</td>
<td>Symmetry / Insulation</td>
</tr>
</tbody>
</table>
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

TRP channels 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