FERRONEMATICS: TECHNICAL NOTE

Key findings of the model:

- The control parameter is the temperature, and they observe a transition form CV-type topologies to L-type topologies as function of this parameter. In particular, as the temperature decreased, the droplets grew, and the polar topology transitioned from the CV-type to the L-type structure.
- On the other hand, by comparing droplets' free energy landscapes, they were able to prove that elastic anisotropy minimally affects polarization topology, which implies that a one single-elastic-approximation is enough for describing the transition.
- So, what are the core elements for the transition?

The free energy is taken from [1]

$$
\begin{aligned}
f = & \frac{K_{11}}{2}\left(\nabla \cdot \mathbf{N}\right)^2 + \frac{K_{22}}{2}\left(\mathbf{N} \cdot \nabla \times \mathbf{N}\right)^2 + \frac{K_{33}}{2}\left(\mathbf{N} \times \nabla \times \mathbf{N}\right)^2 \\
& + \frac{\tau_1}{2}\mathbf{P}^2 + \frac{\tau_2}{2}\mathbf{P}^4 + \frac{h}{2}\left(\nabla \mathbf{P}\right)^2 - \gamma\left(\nabla \cdot \mathbf{N}\right)\mathbf{N} \cdot \mathbf{P} - \frac{1}{2}\mathbf{P} \cdot \mathbf{E}_d .
\end{aligned}
$$

On the other hand, the surface anchoring is given by

$$
f_s = \frac{1}{2}W_Q\left[1 - \left(\mathbf{n} \cdot \mathbf{R}_0\right)^2\right] - W_P\left[\mathbf{n} \cdot \mathbf{R}_0 - 1\right].
$$

Now, considering a linear coupling between the nematic order parameter and the polarization, i.e., $\mathbf{P} = P_0\mathbf{N}$, where $\mathbf{N} = s\mathbf{n}$, we have the bulk free energy, without taking into consideration the depolarization effect, is given by

$$
\begin{aligned}
f = & \frac{K_{11}}{2}\left(\nabla \cdot \mathbf{N}\right)^2 + \frac{K_{22}}{2}\left(\mathbf{N} \cdot \nabla \times \mathbf{N}\right)^2 + \frac{K_{33}}{2}\left(\mathbf{N} \times \nabla \times \mathbf{N}\right)^2 \\
& + \frac{\tau_1}{2}P_0^2\mathbf{N}^2 + \frac{\tau_2}{2}P_0^4\mathbf{N}^4 + \frac{h}{2}P_0^2\left(\nabla \mathbf{N}\right)^2 - \gamma P_0\left(\nabla \cdot \mathbf{N}\right)\mathbf{N} \cdot \mathbf{N}.
\end{aligned}
$$

$$
\begin{aligned}
f = & \frac{K_{11}}{2}\frac{1}{\xi^2}\left(\nabla \cdot \mathbf{N}\right)^2 + \frac{K_{22}}{2}\frac{1}{\xi^2}\left(\mathbf{N} \cdot \nabla \times \mathbf{N}\right)^2 + \frac{K_{33}}{2}\frac{1}{\xi^2}\left(\mathbf{N} \times \nabla \times \mathbf{N}\right)^2 \\
& + \frac{\tau_1}{2}P_0^2\mathbf{N}^2 + \frac{\tau_2}{2}P_0^4\mathbf{N}^4 + \frac{h}{2}P_0^2\frac{1}{\xi^2}\left(\nabla \mathbf{N}\right)^2 - \gamma P_0\frac{1}{\xi}\left(\nabla \cdot \mathbf{N}\right)\mathbf{N} \cdot \mathbf{N}.
\end{aligned}
$$

$$
\begin{aligned}
\int_\Omega f = & \xi^2\left(\frac{K_{11}}{2}\frac{1}{\xi^2}\left(\nabla \cdot \mathbf{N}\right)^2 + \frac{K_{22}}{2}\frac{1}{\xi^2}\left(\mathbf{N} \cdot \nabla \times \mathbf{N}\right)^2 + \frac{K_{33}}{2}\frac{1}{\xi^2}\left(\mathbf{N} \times \nabla \times \mathbf{N}\right)^2\right) \\
& + \xi^2\left(\frac{\tau_1}{2}P_0^2\mathbf{N}^2 + \frac{\tau_2}{2}P_0^4\mathbf{N}^4 + \frac{h}{2}P_0^2\frac{1}{\xi^2}\left(\nabla \mathbf{N}\right)^2 - \gamma P_0\frac{1}{\xi}\left(\nabla \cdot \mathbf{N}\right)\mathbf{N} \cdot \mathbf{N}\right).
\end{aligned}
$$

$$\int_\Omega f = \frac{K_{11}}{2}\left(\nabla\cdot\mathbf{N}\right)^2 + \frac{K_{22}}{2}\left(\mathbf{N}\cdot\nabla\times\mathbf{N}\right)^2 + \frac{K_{33}}{2}\left(\mathbf{N}\times\nabla\times\mathbf{N}\right)^2$$
$$+\frac{\tau_1}{2}P_0^2\xi^2\mathbf{N}^2 + \frac{\tau_2}{2}P_0^4\xi^2\mathbf{N}^4 + \frac{h}{2}P_0^2\left(\nabla\mathbf{N}\right)^2 - \gamma P_0\xi\left(\nabla\cdot\mathbf{N}\right)\mathbf{N}\cdot\mathbf{N}.$$

One Constant Approximation. In the one constant approximation the Fredericks free energy reduces to $\frac{1}{2}K_1\left(\nabla\mathbf{N}\right)^2$, thus it follows that

$$f = \frac{K_{11}}{2}\left(\nabla\cdot\mathbf{N}\right)^2 + \frac{\tau_1}{2}\mathbf{P}^2 + \frac{\tau_2}{2}\mathbf{P}^4 + \frac{h}{2}\left(\nabla\mathbf{P}\right)^2 - \gamma\left(\nabla\cdot\mathbf{N}\right)\mathbf{N}\cdot\mathbf{P},$$

again, without taking the depolarization effect. We could write the above free energy in terms of just $\mathbf{N}$ as follows

$$f = \frac{K_{11}}{2}\left(\nabla\cdot\mathbf{N}\right)^2 + \frac{\tau_1 P_0^2}{2}\mathbf{N}^2 + \frac{\tau_2 P_0^4}{2}\mathbf{N}^4 + \frac{hP_0^2}{2}\left(\nabla\mathbf{N}\right)^2 - \gamma P_0\left(\nabla\cdot\mathbf{N}\right)\mathbf{N}\cdot\mathbf{N},$$

Now, let's choose K_{11} for rescaling and ξ for rescaling and dimensionless purposes respectively

$$f' = \frac{1}{2}\left(\nabla\cdot\mathbf{N}\right)^2 + \frac{1}{2}\tau_1'\mathbf{N}^2 + \frac{1}{2}\tau_2'\mathbf{N}^4 + \frac{1}{2}h'\left(\nabla\mathbf{N}\right)^2 - \gamma'\left(\nabla\cdot\mathbf{N}\right)\mathbf{N}\cdot\mathbf{N},$$

where the constants are given by

$$\tau_1' = \frac{\tau_1 P_0^2}{K_{11}}\xi^2, \tau_2' = \frac{\tau_2 P_0^4}{K_{11}}\xi^2, h' = \frac{hP_0^2}{K_{11}}, \gamma' = \frac{\gamma P_0}{K_{11}}\xi.$$

The numerical values of the constants are given by

Parameters	Values	Rescaled Values
K_{11}	$10^{-12}N$	
K_{33}	$1.2\times10^{-12}N$	
P_0	$0.045\frac{C}{m^2}$	
τ_1	$-10^3\frac{Jm}{C}$	
τ_2	$9.88\times10^5\frac{Jm^5}{C^4}$	
γ	$10^{-4}V$	
ε	$10^{-7}\frac{F}{m}$	
β	10^{-5}	
W_Q	$1\times10^{-6}\frac{J}{m^2}$	
W_P	$1\times10^{-6}\frac{J}{m^2}$	
h	$10^{-10}Jm^3C^{-2}$	

And from this we can compute the numerical values as follows

$$\tau_1' = -\frac{\left(10^3\right)\left(0.045\right)^2}{\left(10^{-12}\right)}\xi^2,$$
$$\tau_2' = \frac{\left(9.88 \times 10^5\right)\left(0.045\right)^4}{\left(10^{-12}\right)}\xi^2,$$
$$h' = \frac{\left(10^{-10}\right)\left(0.045\right)^2}{\left(10^{-12}\right)},$$
$$\gamma' = \frac{\left(10^{-4}\right)\left(0.045\right)}{\left(10^{-12}\right)}\xi$$

therefore, we have

$$\tau_1' = -2.025 \times 10^{12}\xi^2$$
$$\tau_2' = 4.05142 \times 10^{11}\xi^2$$
$$h' = 0.2025$$
$$\gamma' = 4.5 \times 10^6\xi$$

and if we choose $\xi = 1 \times 10^{-6}$, then we have

$$\tau_1' = -2.025$$
$$\tau_2' = 0.405142$$
$$h' = 0.2025$$
$$\gamma' = 4.5$$

sand for the surface terms we have the following expressions for the dimensionless parameters

$$\omega_Q' = \frac{W_Q}{K_{11}}\xi, \quad \omega_P' = \frac{W_P}{K_{11}}\xi$$

It makes sense to consider ξ as the size of the domain.

For the CV type here are some numerical values for the phenomenological parameters;

$$K_{11} = 10^{-12}N,$$

What about the Depolarization Effect?

By definition, the depolarization effect occurs when the electric field inside a material is reduced due to the alignment of dipoles within the material, which produce their own opposing field. For the CV-type we have the following expression for the depolarization

$$f = \frac{1}{2}P_{\text{eff}}\cos\left(b + kr\right)\left[\frac{1}{r} + \frac{\beta P_{\text{eff}}\cos\left(b + kr\right)}{\epsilon}\right],$$

Under the one constant approximation we have the following free energy

$$f' = K_1' \left(\nabla \cdot \mathbf{N}\right)^2 + \tau_1' \mathbf{N}^2 + \tau_2' \mathbf{N}^4 + h' \left(\nabla \mathbf{N}\right)^2 - \gamma' \left(\nabla \cdot \mathbf{N}\right) \mathbf{N} \cdot \mathbf{N},$$

with the same dimensionless constants as in the full model.

Question: Is there a special boundary condition for the electric field—already know that P is tangent to the boundary.

Results So Far:

Landau:

To-Do: $+\frac{\tau_1}{2} P_0^2 \mathbf{N}^2 + \frac{\tau_2}{2} P_0^4 \mathbf{N}^4$

(1) **Landau only (Done)**
(2) **Landau + $|\nabla P|^2$: We observe some kind of.**
(3) **Landau + $|\nabla P|^2$ + Anchoring: We observe some kind of structural transition.**
(4) Landau + $|\nabla P|^2$+Frank
(5) Everything
(6) Learn that solving Poisson is equivalent to minimizing $\int \left(|\nabla \phi|^2 - \rho \phi \right) d^n x$

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for i in
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To-Do:

Use Mathematica to work out the equilibrium value of P as a function of T just for the Landau Expansion (using dimensionless parameters).

References

[1] Rosseto, Michely P., and Jonathan V. Selinger. "Theory of the splay nematic phase: single versus double splay." Physical Review E 101, no. 5 (2020): 052707.