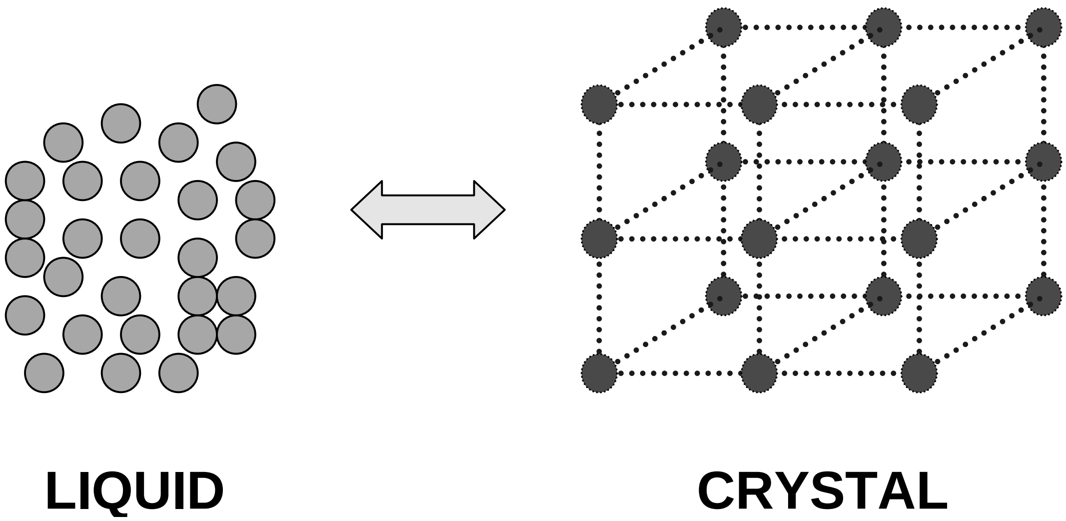
Measurement of liquid crystal surface anchoring by molecular simulation

DENIS ANDRIENKO
GUIDO GERMANO
MICHAEL P. ALLEN

H.H. Wills Physics Laboratory, University of Bristol,
Royal Fort, Tyndall Avenue, Bristol BS8 1TL, United Kingdom

- What is a liquid crystal.
- Anchoring phenomena. Why is it so important?
- Computer simulation. State of art in the surface effects.
- Director fluctuations.
- Confined LCs. Influence of confinement on the fluctuation modes.
- Simulation data and fitting.
- Final remarks: advantages and disadvantages of the method.

What is a liquid crystal?

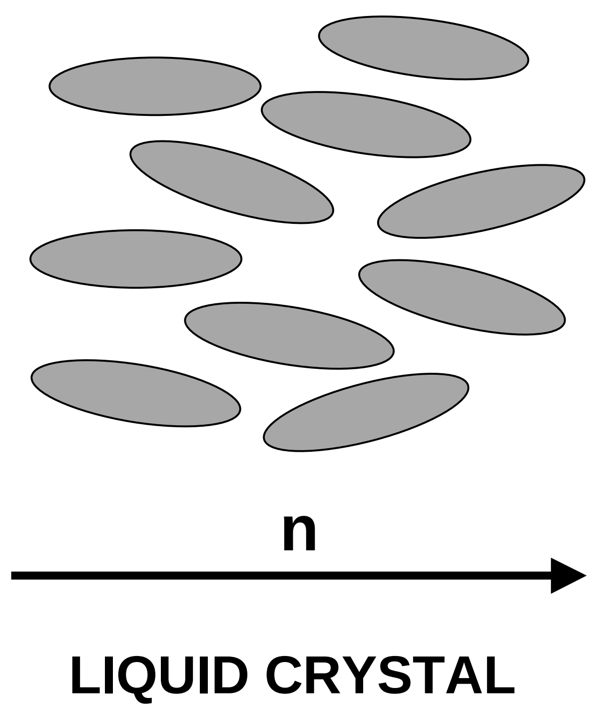


Orientational degrees of freedom

Anisotropic objects

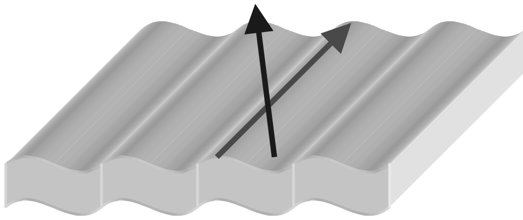
No positional order

Orientational order
n – director
Q – order parameter



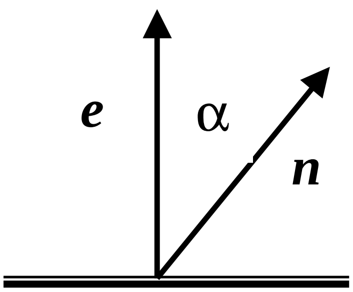
Surface anchoring

Berreman's model of anchoring



$$F_{surface} = -\frac{1}{2} W \int dS \cos^2 \alpha$$

Rapini potential



$$F_{surface} = -\frac{1}{2} W \int dS \left(\boldsymbol{ne} \right)^2$$

W anchoring energy

$\boldsymbol{e}$ easy axis

Experimental methods:

- Measure surface director deviations in an external field. Involve rather complicated optical setups.
- Test the entire liquid crystal cell and cannot provide satisfactory description of a thin interface region.

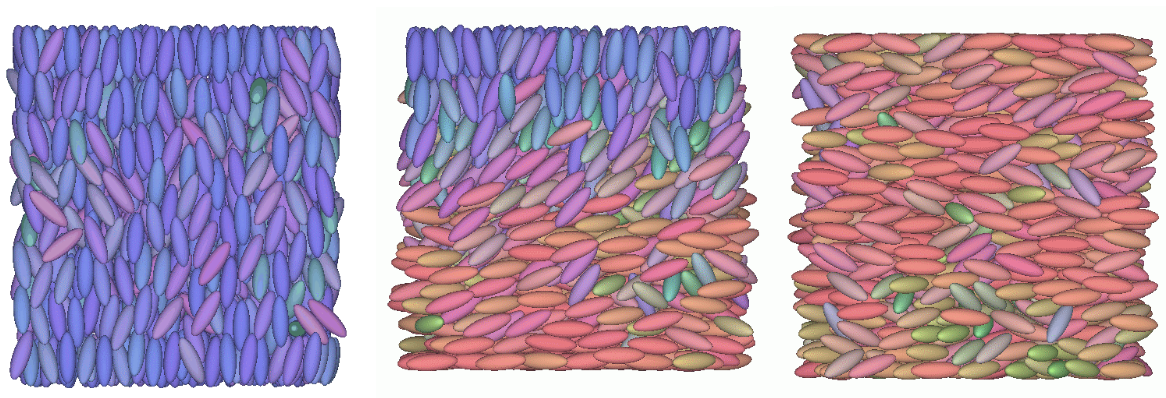
Theoretical investigations:

- Continuous phenomenological theory has divergent surface terms
- Strong subsurface deformations

Computer Simulation

Why? - Can test orientational ordering, density profiles on a molecular scale.

What has been done? - Various surface potentials have been proposed: Lenard–Jones interaction, Gay-Berne type interaction, etc.



Homeotropic Hybrid Planar

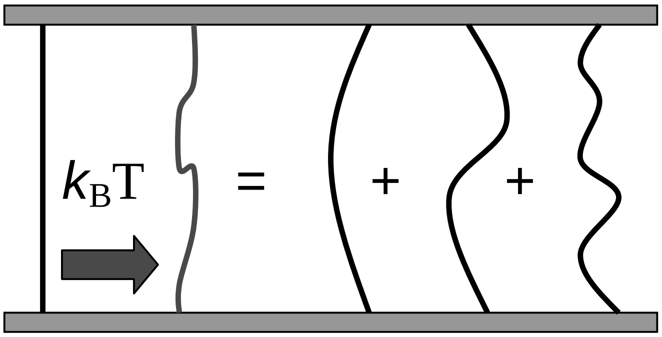
But! - Most of the works do not characterise aligning surfaces (or potentials) using well-established parameters: e.g. anchoring energy.

Reason? - Lack of reliable methods to measure these parameters by computer simulation.

HOW?

Director fluctuations

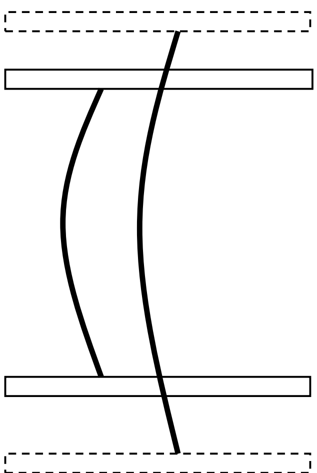
Strong anchoring



$$\delta \boldsymbol{n}(\boldsymbol{r}) = \sum_{\boldsymbol{q}} \delta \boldsymbol{n}(\boldsymbol{q}) \exp i(\boldsymbol{qr})$$

$$q_z = \frac{\pi}{L} n, \quad n = 1,2,...$$

Weak anchoring

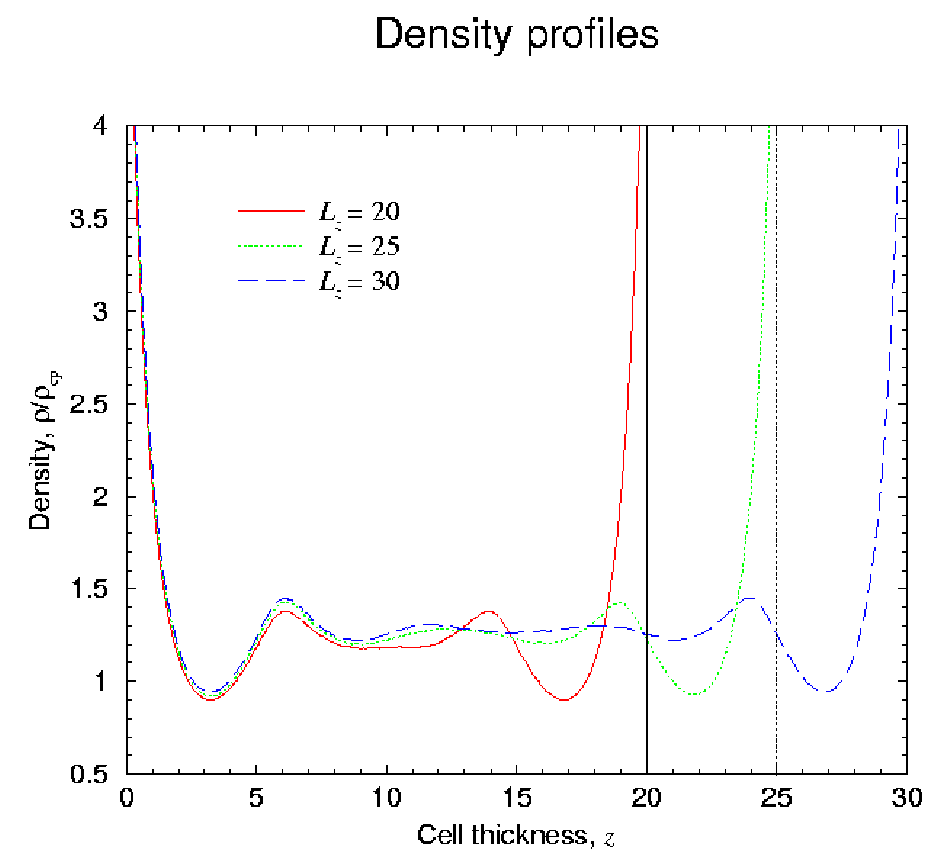


✓ q_z spectrum depends on the anchoring parameter WL/K.

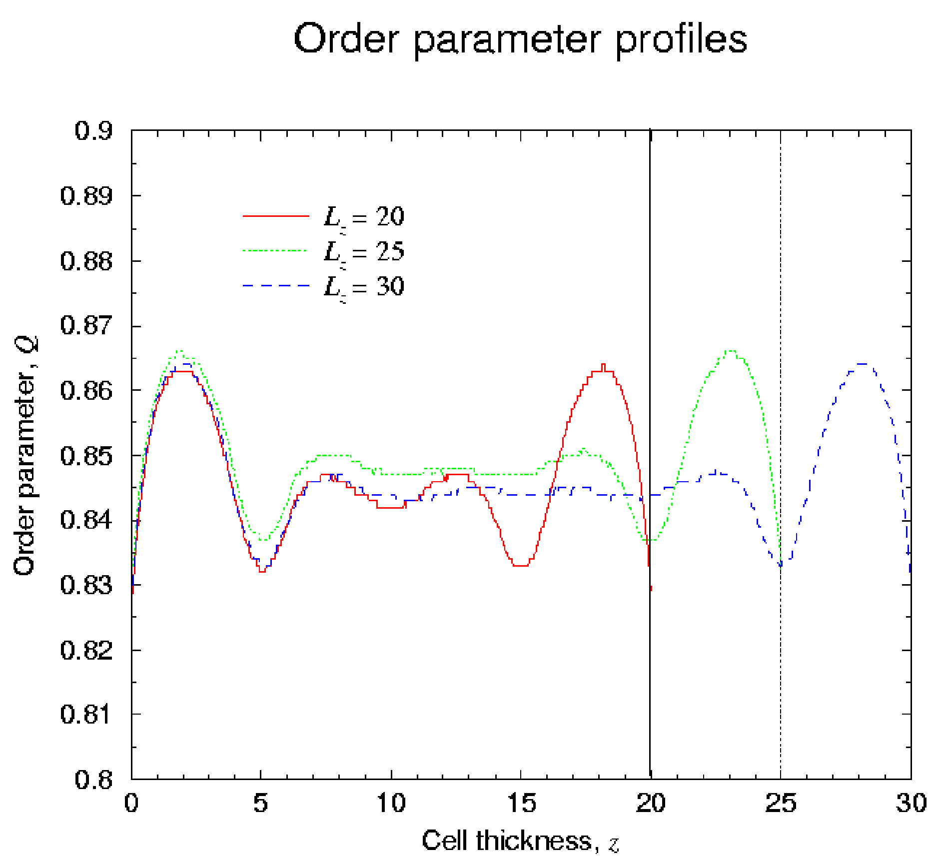
✓ Amplitudes of the director fluctuations depend on WL/K.

CONCLUSION

If we can measure director fluctuations we can measure anchoring strength!

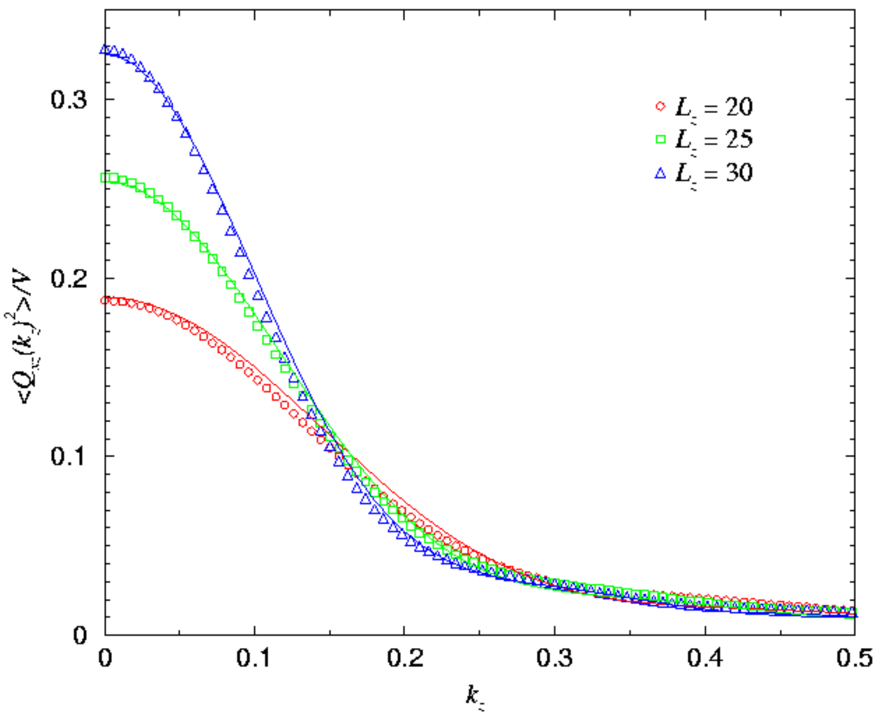


Density profiles
$L_z = 20$
$L_z = 25$
$L_z = 30$
Density, ρ/ρ_{cp}
Cell thickness, z



Order parameter profiles
$L_z = 20$
$L_z = 25$
$L_z = 30$
Order parameter, Q
Cell thickness, z

Order tensor fluctuations



Advantages and disadvantages

The most sensitive to the surfaces are large time- and length-scale fluctuations. Therefore, one needs **long runs** to obtain suitable thermodynamic averages**.**

It is not possible to measure large values of the anchoring parameter *WL*/*K*, so we need **reasonably thin cells**. However, we are limited from the side of small *L* since relaxation times of fluctuations increase and again we are not able to reach thermodynamic averages.

Also one has to remember that the ***bulk*** region should be **sufficiently large** compared to the ***interfacial*** region. Only in this case we can assume that the scalar order parameter Q in the liquid crystal bulk is constant for large-scale fluctuation modes.