

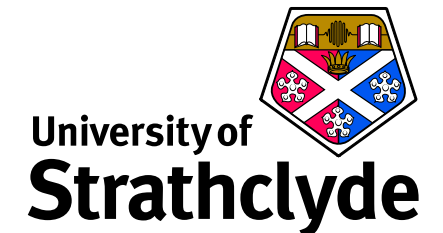
A MODEL OF DUAL FREQUENCY NEMATIC LIQUID CRYSTALS

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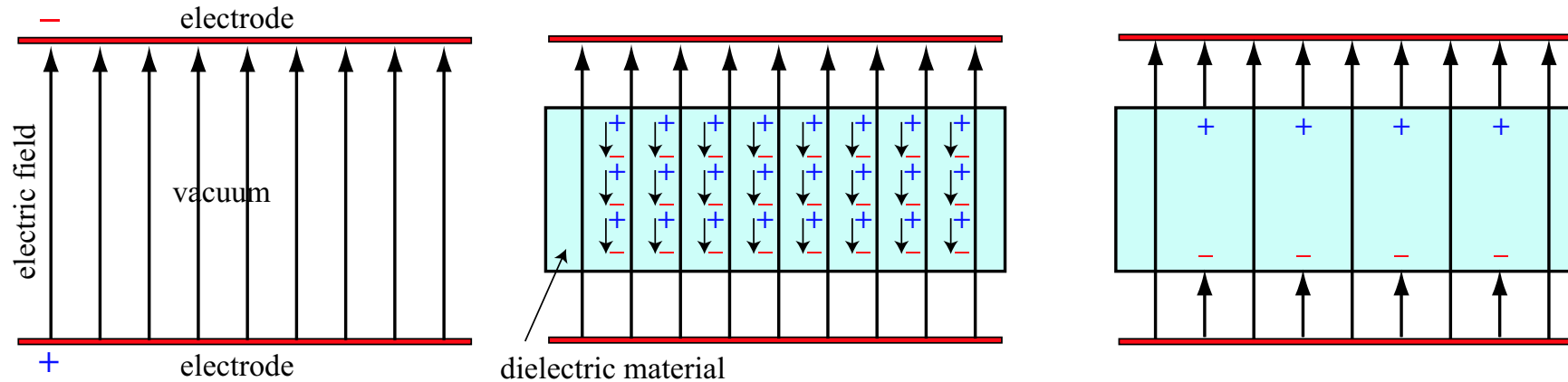
funding: EPSRC



Motivation

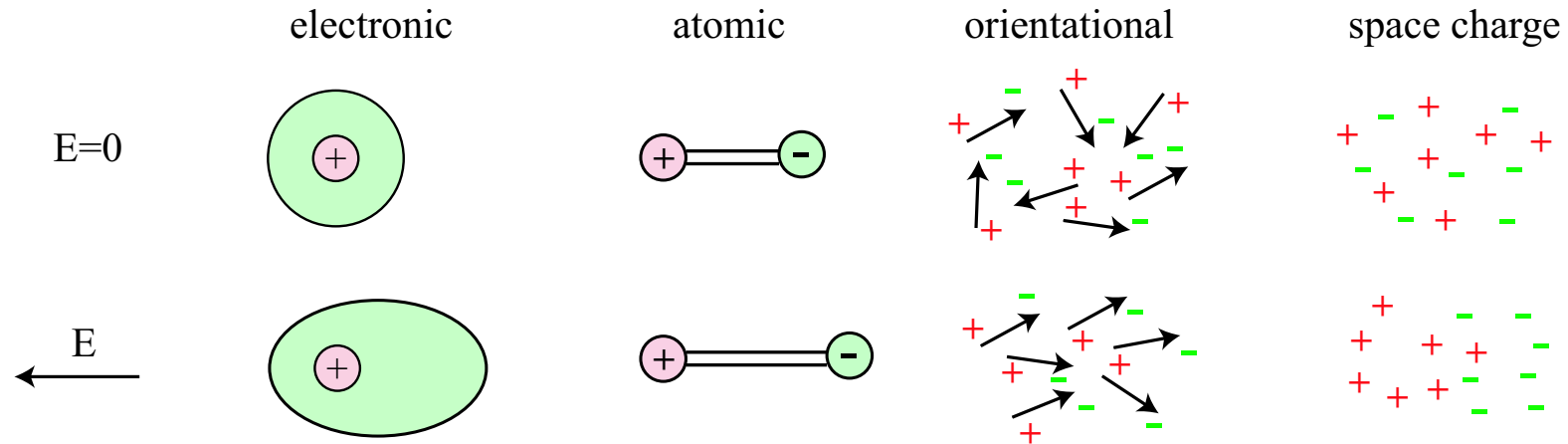
- Development of a general model of dielectric relaxation in liquid crystals.
- Dual frequency materials will give increased functionality, more control over orientation.
- Ability to switch on and off, rather than relying on director relaxation, increases switching speed.
- Are the problems with dual frequency materials identified in the late 70s still a barrier for exploitation?

Dielectric materials



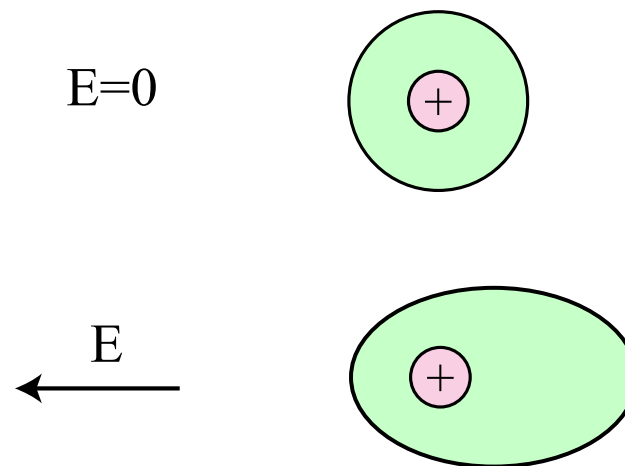
- Electric field induces dipoles in a dielectric material.
- These dipoles create a *depolarisation field* within the dielectric.
- This causes a reduction in the electric field within the dielectric.
- This means the charge storage capacity (capacitance) of a dielectric is greater than vacuum.
- Dielectric permittivity is defined as the ratio of capacitance of the dielectric filled capacitor to the empty capacitor.

Induced polarisation



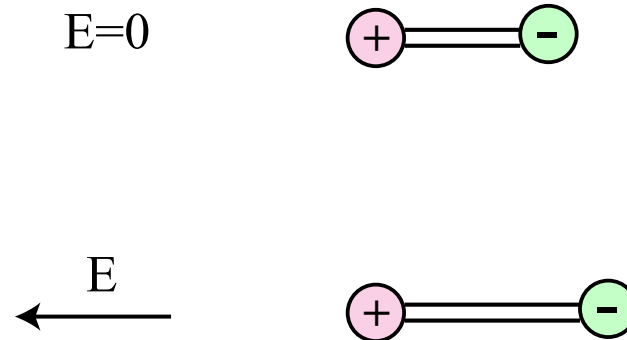
- In a dielectric, the dipoles may be induced in a number of ways.
- The total polarisation is the sum of these contributions.
- The polarisation is related to the applied field through the *dielectric susceptibility* χ :
 $\mathbf{P} = \epsilon_0 \chi \mathbf{E}$.

Induced polarisation I: Electronic



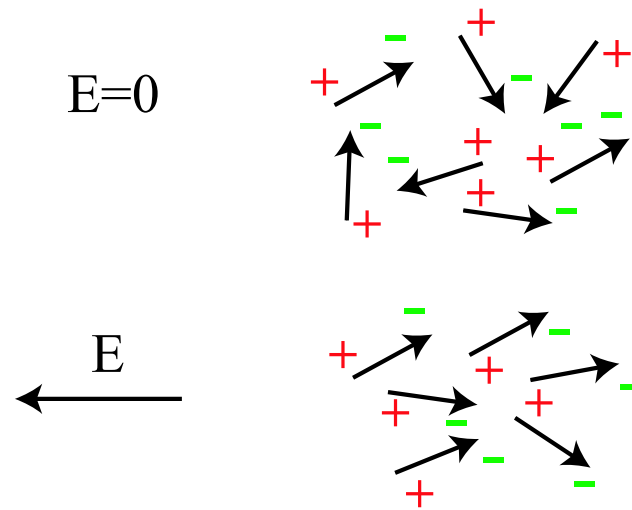
- Dipoles caused by displacement of the electrons with respect to the atomic nucleus.

Induced polarisation II: Atomistic



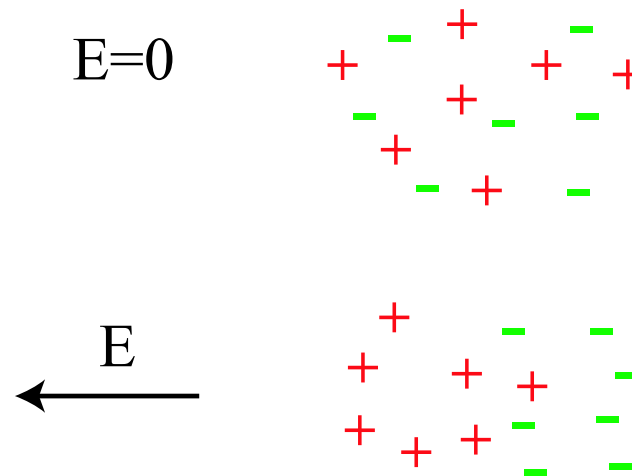
- Different atoms in a molecule may share their electrons asymmetrically causing the electron cloud to be distorted.
- This means atoms will acquire charges of opposite polarity.
- An external field will act on these charges and change the equilibrium positions of the atoms.

Induced polarisation III: Orientational



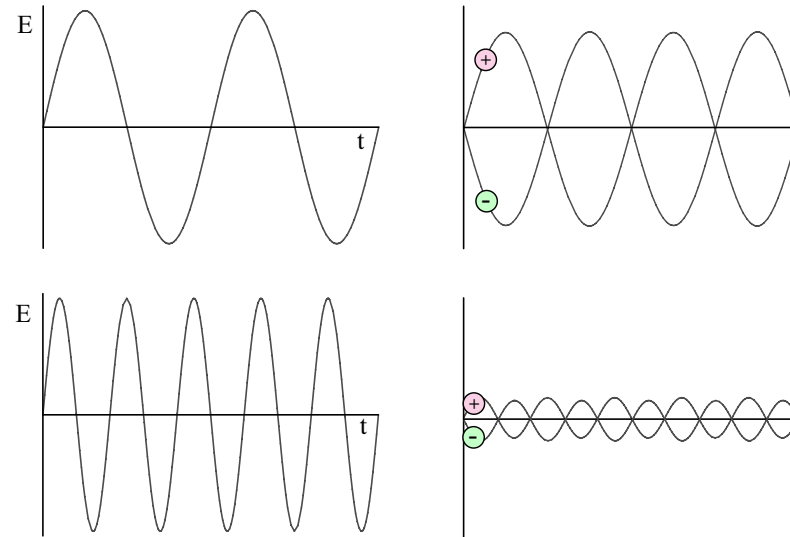
- Each molecule contains a permanent molecular dipole.
- Application of a field will align these dipoles creating a polarisation.

Induced polarisation IV: Space charge



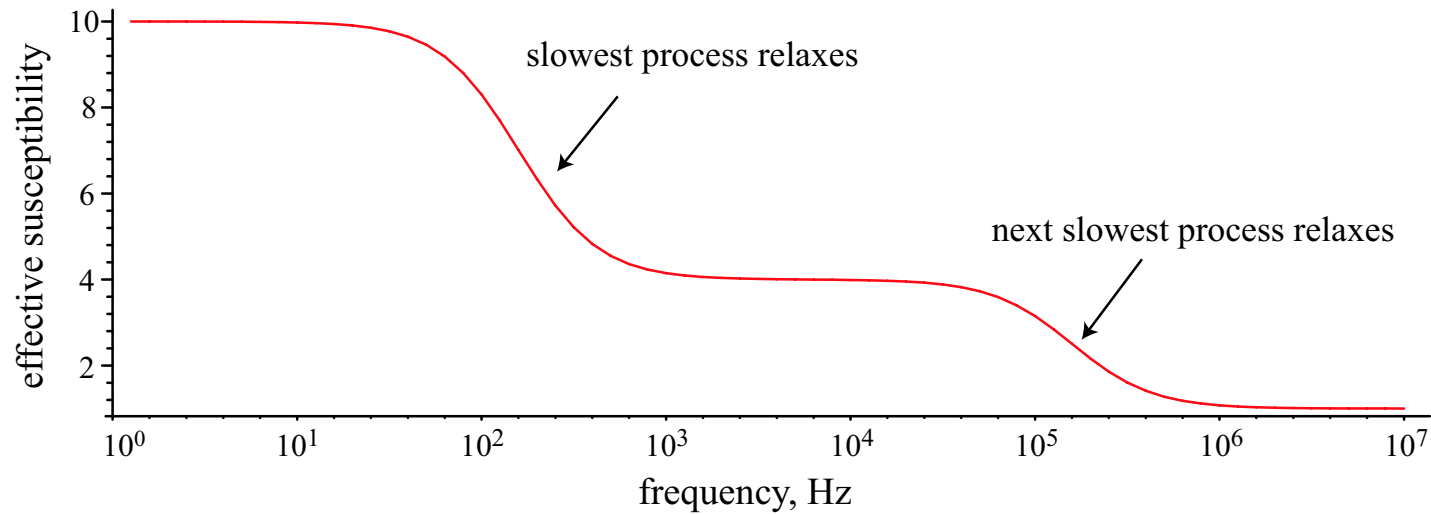
- Charge carriers may be present in the dielectric (i.e. ions) which can move through the material.
- An applied electric field will cause ions to migrate towards the electrodes.
- We will neglect this effect although ions can easily be added into our model.

Periodic excitation



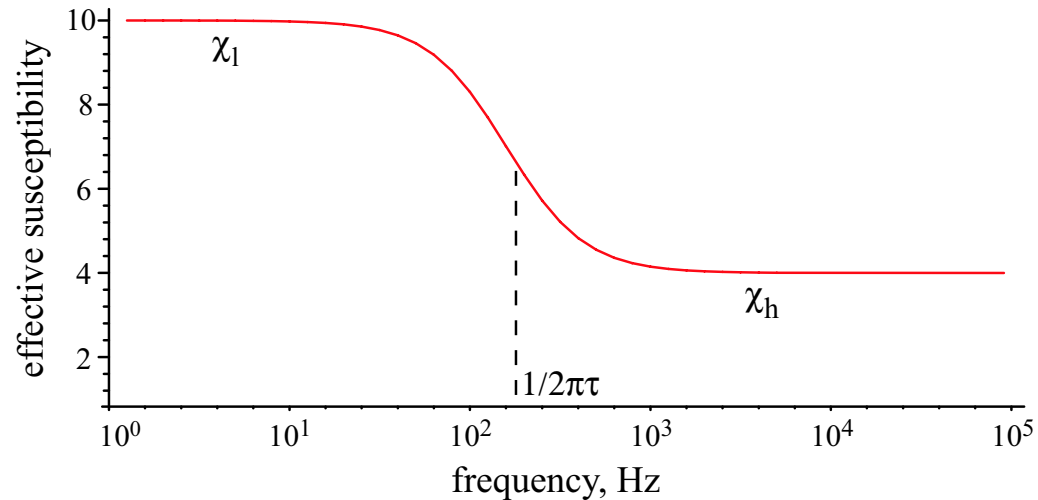
- At low frequencies, the induced polarisation will follow the oscillating field, possibly with some phase delay.
- At high enough frequencies, resistance to the formation of the polarisation means that the polarisation formation is not sufficiently fast to follow the field. The amplitude of the induced polarisation is reduced.
- A decrease in induced polarisation causes a decrease in capacitance and therefore a decrease in dielectric susceptibility χ .
- This is *dielectric relaxation*.

Dielectric relaxation



- Each of the mechanisms for inducing polarisation has a characteristic time constant.
- When the frequency of the applied field increases beyond each characteristic time, a process will be unable to follow the field and relaxation of a mode will occur.

Debye process



Debye realised this process follows a relatively simple rule.

$$\chi = \chi_h + \frac{\chi_l - \chi_h}{1 + (2\pi f)^2 \tau^2}$$

where χ_h and χ_l are the high and low frequency asymptotic values of χ , and τ is the characteristic time for the process which forms the induced polarisation.

Debye process

$$\chi = \chi_h + \frac{\chi_l - \chi_h}{1 + (2\pi f)^2 \tau^2}$$

- This gives χ as a function of f but what if the applied field is not sinusoidal?
- We could find the Fourier series of the waveform and then calculate an effective χ . But this may be a lengthy calculation, particularly for step/pulse waveforms.
- The alternative is to model the induced polarisation directly.

Lorentz oscillator

We will model each of the induced polarisations using the equation for a damped forced oscillator,

$$m \frac{d^2 P}{dt^2} + \gamma \frac{dP}{dt} + kP = F$$

The first term represents the inertial force,
the second is due to frictional forces,
the third is a restoring term which indicates a preference for $P = 0$ in an unforced state,
the last term is the external forcing term.

In fact, if the relaxation process is non-resonant (as the molecular reorientation process is)
 $m = 0$.

Model

- We will assume that each of the dipoles caused by dielectric interaction can be represented by a Lorentz oscillator.
- We can decompose the polarisations into components parallel and perpendicular to the nematic director $\mathbf{n} = (\cos \theta, 0, \sin \theta)$.
- We will then assume that all processes except rotation about the short axis of the molecule ($P_{||}^r$) are extremely fast.
- This means that, for the frequencies we will apply to our cell, rotation about the long molecular axis (P_{\perp}^r), electronic ($P_{||}^e, P_{\perp}^e$) and atomistic processes ($P_{||}^a, P_{\perp}^a$) will exactly follow the applied field.

Equations: polarisation

Total polarisation, either parallel and perpendicular to the director, is the sum of contributions from reorientation, electronic and atomistic effects,

$$\begin{aligned}P_{\parallel} &= P_{\parallel}^r + P_{\parallel}^e + P_{\parallel}^a \\P_{\perp} &= P_{\perp}^r + P_{\perp}^e + P_{\perp}^a\end{aligned}$$

Reorientation about the long molecular axis, electronic and atomistic effects are fast enough to follow the electric field within the dielectric material,

$$\begin{aligned}P_{\perp}^r + P_{\perp}^e + P_{\perp}^a &= \epsilon_0 \chi_{\perp l} E \cos \theta \\P_{\parallel}^e + P_{\parallel}^a &= \epsilon_0 \chi_{\parallel l} E \sin \theta\end{aligned}$$

The polarisation due to rotation about the short molecular axis will be found by solving,

$$\tau \frac{dP_{\parallel}^r}{dt} + P_{\parallel}^r = \epsilon_0 \chi_{\parallel l}^r E \sin \theta$$

Equations: electric field

The electric field in the z direction, within the dielectric, is found using Maxwell's equations,

$$E = -\frac{V}{d} + \frac{1}{\epsilon_0 d} \int_0^d (P_{\parallel} \sin \theta + P_{\perp} \cos \theta) dz - \frac{1}{\epsilon_0} (P_{\parallel} \sin \theta + P_{\perp} \cos \theta)$$

assuming that $V(d) - V(0) = V$.

The displacement field in the z direction is

$$D = \epsilon_0 E + P_{\parallel} \sin \theta + P_{\perp} \cos \theta.$$

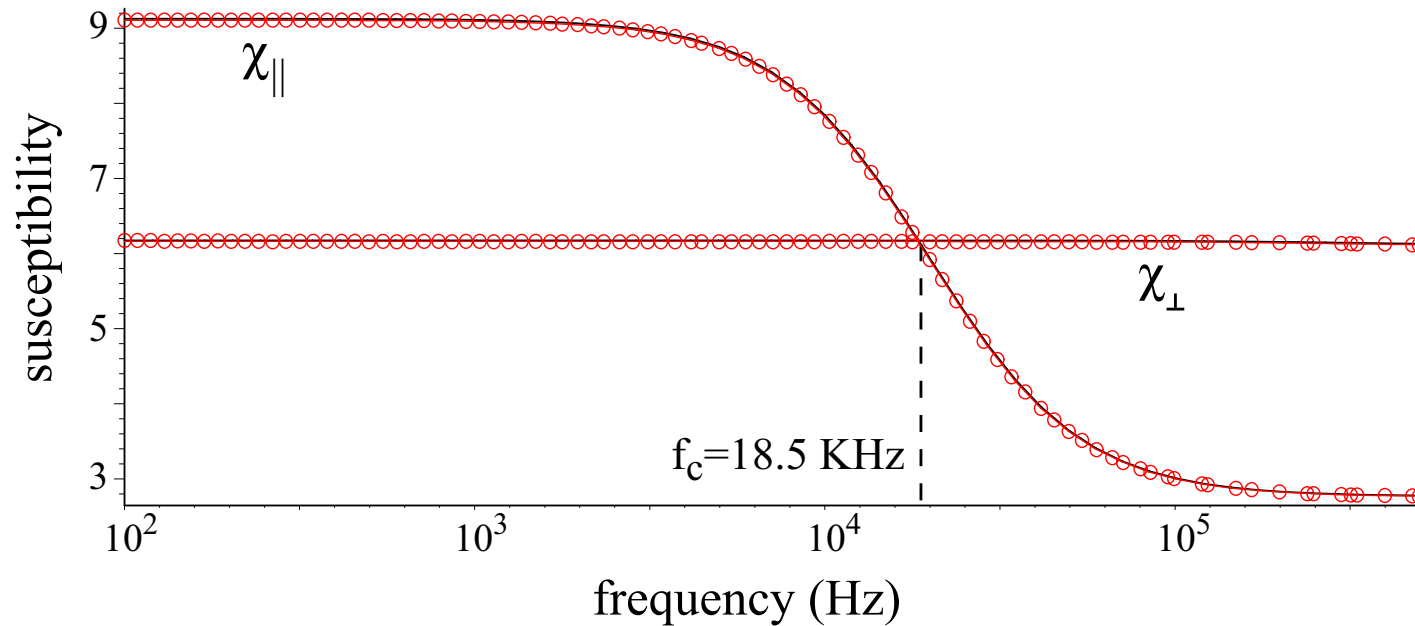
Equations: director

If the director remains in the xz plane, at an angle θ to the horizontal, and we neglect flow effects, θ will satisfy

$$\gamma_1 \frac{\partial \theta}{\partial t} = (K_1 \cos^2 \theta + K_3 \sin^2 \theta) \frac{\partial^2 \theta}{\partial z^2} + \frac{1}{2} (K_3 - K_1) \sin \theta \cos \theta \left(\frac{\partial \theta}{\partial z} \right)^2 + (P_{||} \cos \theta - P_{\perp} \sin \theta) E,$$

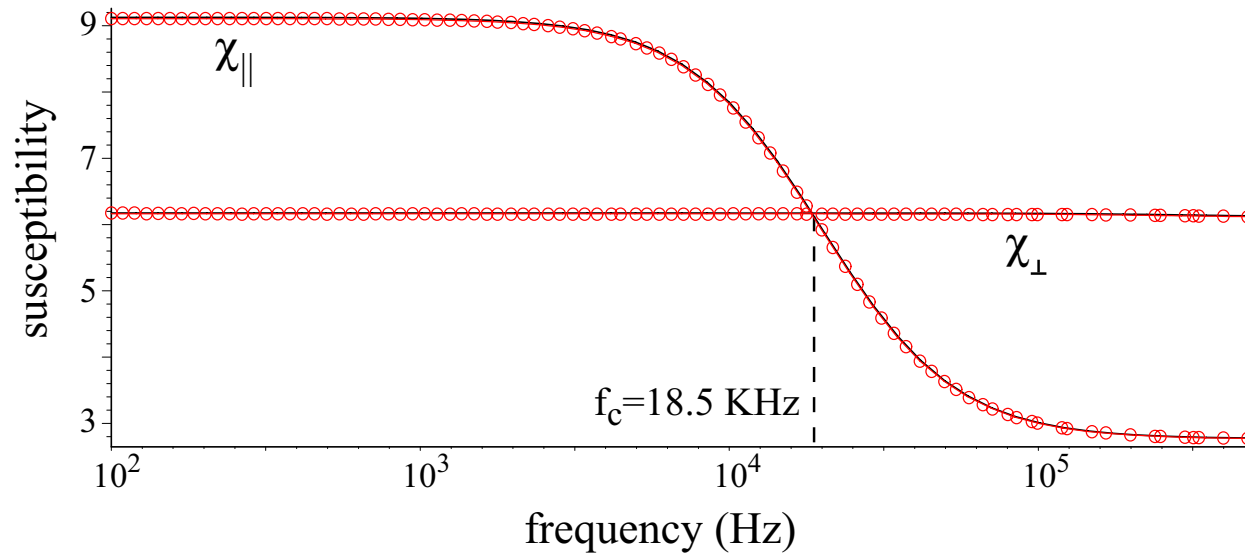
The electric field term derives from the electrostatic free energy density $-\int D dE$.

Fitting experimental data



- Capacitance measurement in a planar cell gives χ_{\perp} .
- Capacitance measurement in a homeotropic cell gives $\chi_{||}$.
- Model (black lines) is fitted to experimental results to give the parameters, $\chi_{||l}^r = 6.36$, $\chi_{||l} = 2.77$, $\chi_{\perp l} = 6.17$, $\tau = 20.05 \times 10^{-6}$ s.
- Fredericks transition experiments give the remaining parameters, $K_1 = 1.49 \times 10^{-11}$ N, $K_3 = 2.0 \times 10^{-11}$ N, $\gamma_1 = 0.05$ Pas.

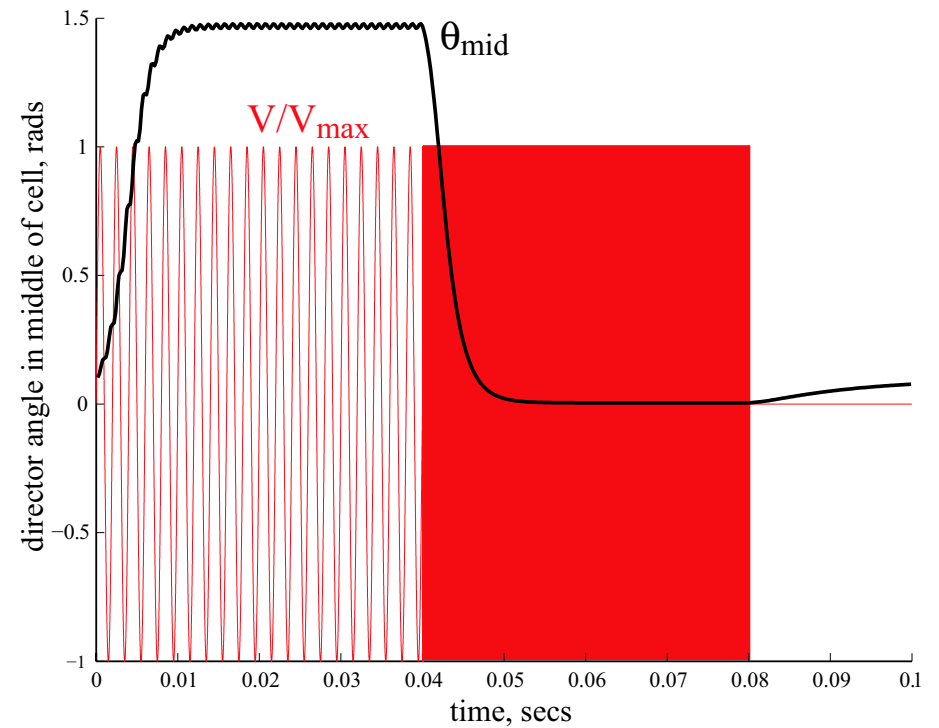
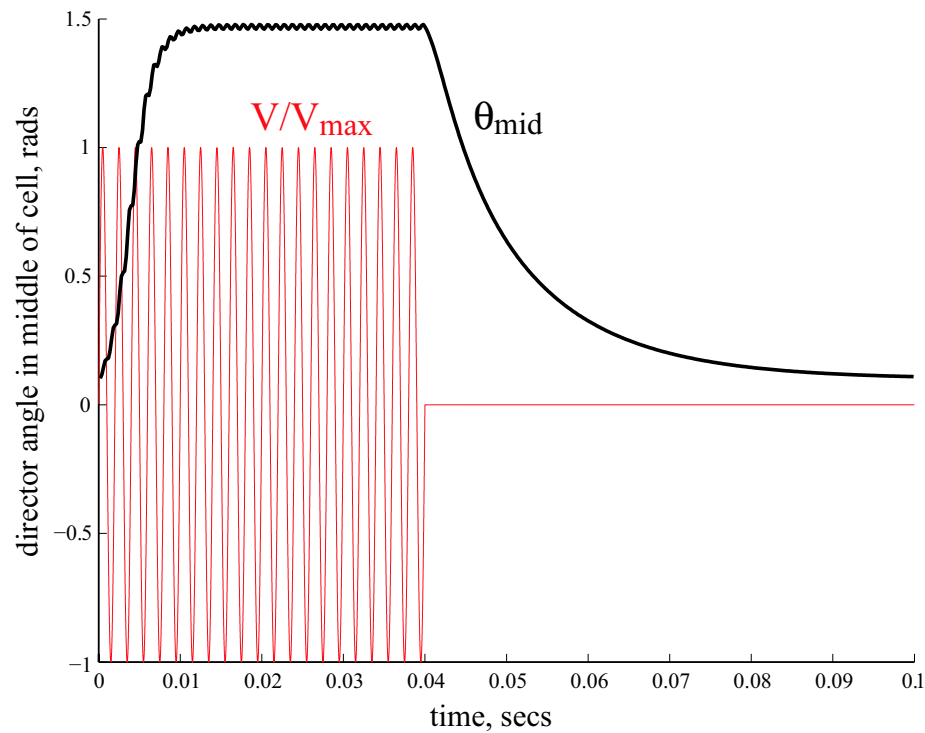
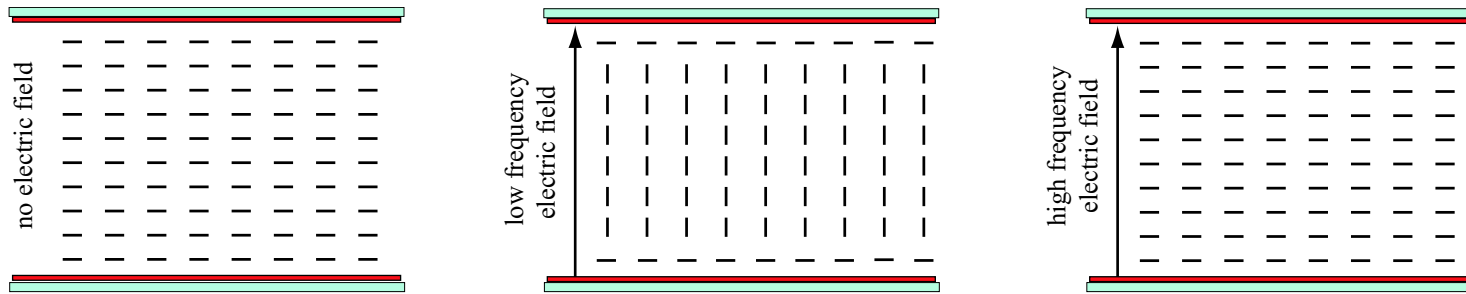
Dual frequency switching



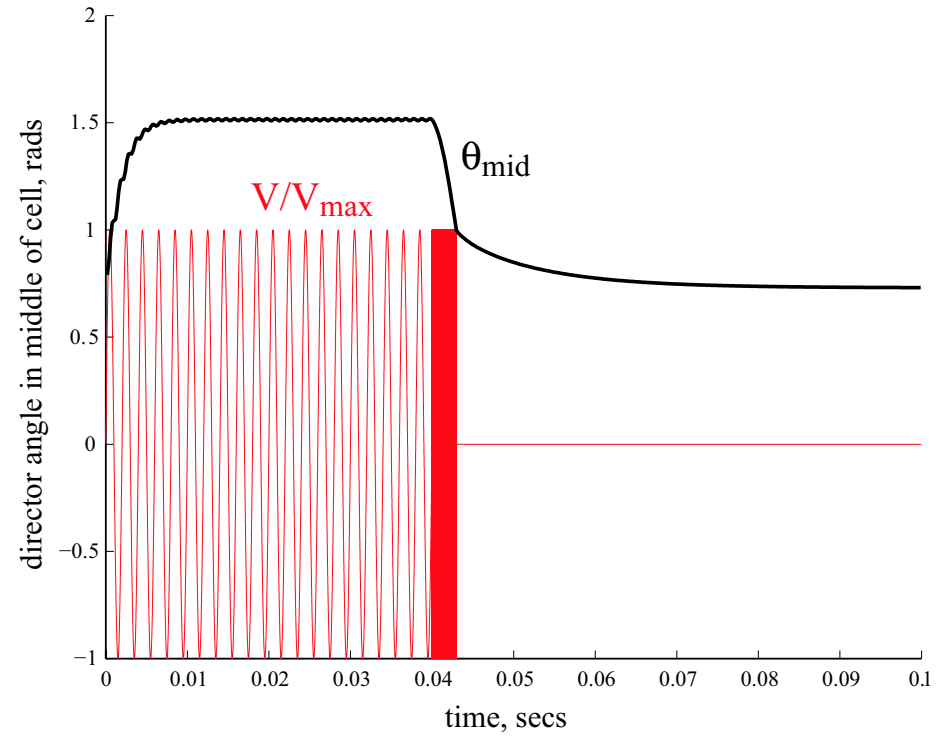
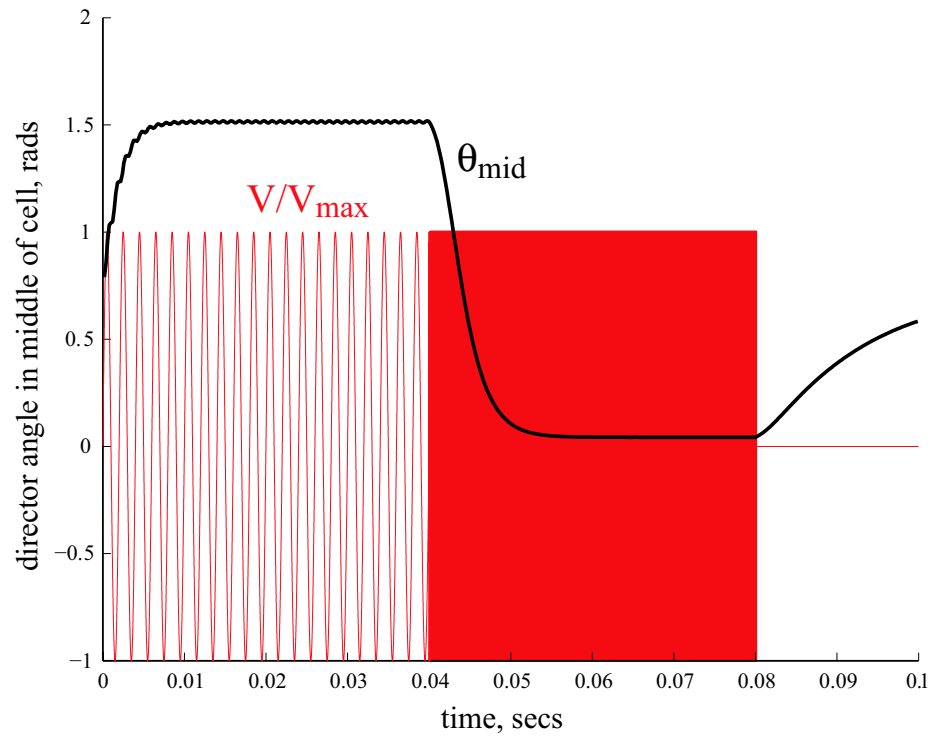
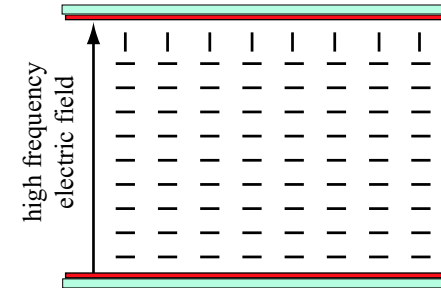
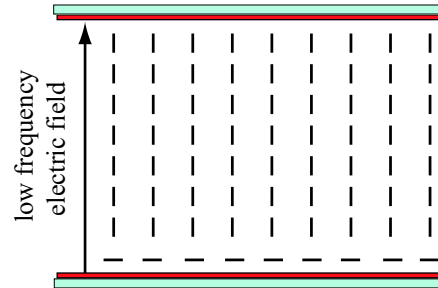
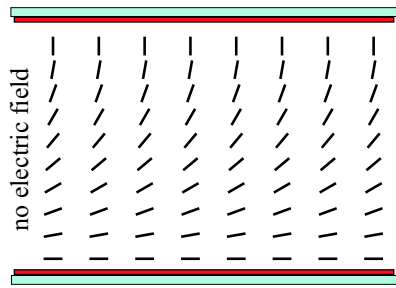
- For low frequency fields the rotation about the short molecular axis has not relaxed. The parallel susceptibility is larger than the perpendicular susceptibility and $\Delta\chi = \chi_{\parallel} - \chi_{\perp} > 0$ ($\Delta\epsilon > 0$).
- For high frequency fields the rotation about the short molecular axis has relaxed. The parallel susceptibility is now smaller than the perpendicular susceptibility and $\Delta\chi < 0$ ($\Delta\epsilon < 0$).

Freedericksz cell

- 5 volts, cell thickness $3\ \mu\text{m}$, pretilt $0.1\ \text{rads}$, low frequency $f = 500\ \text{Hz}$, high frequency $f = 50\ \text{KHz}$

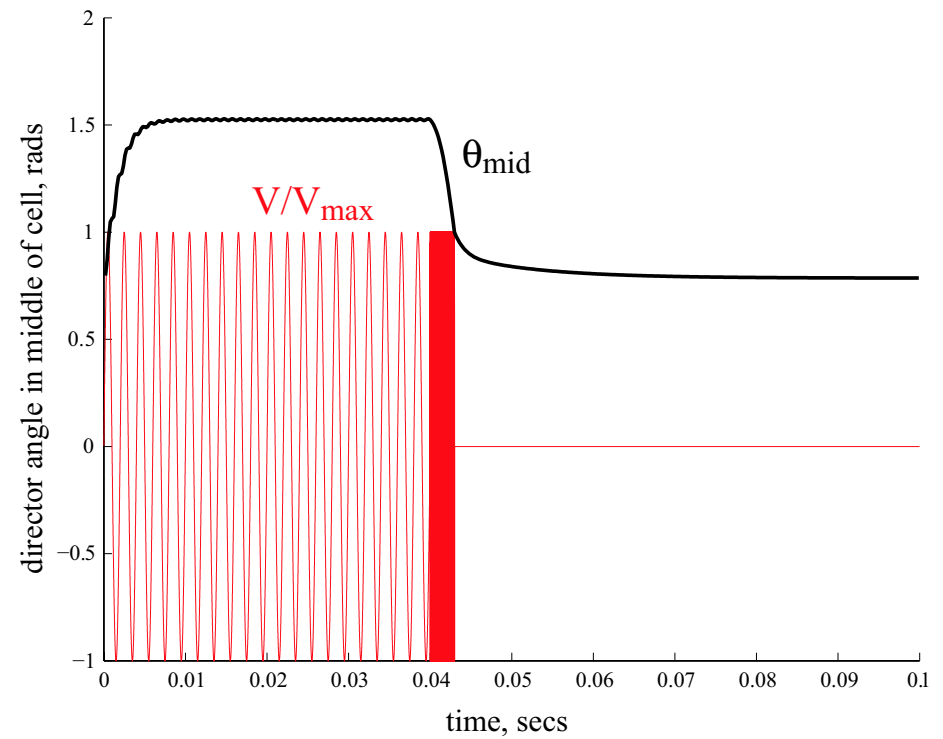
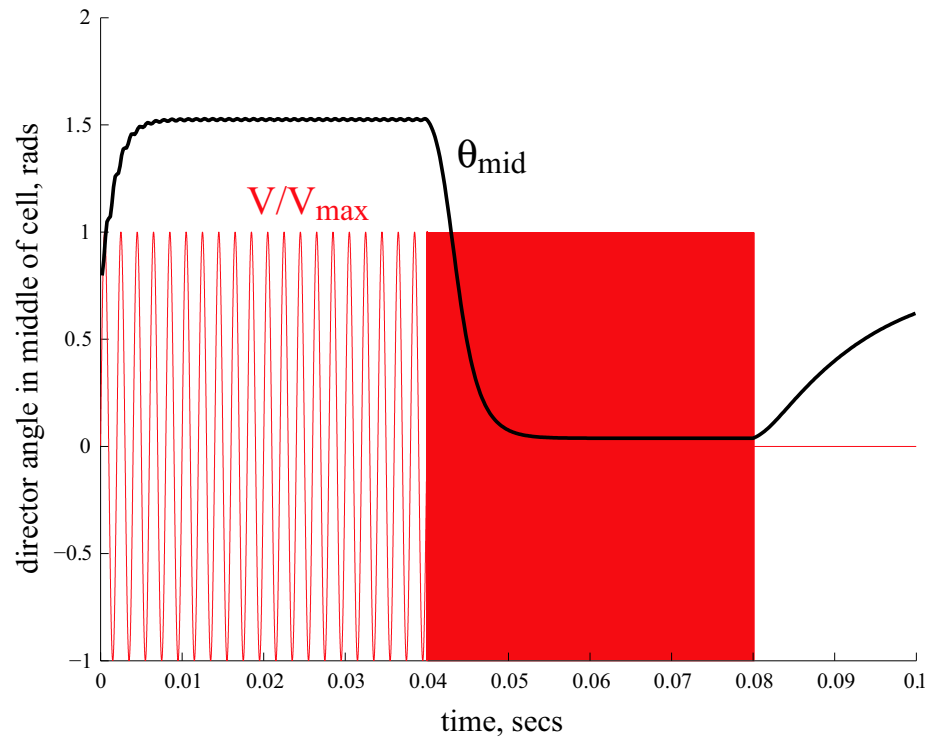
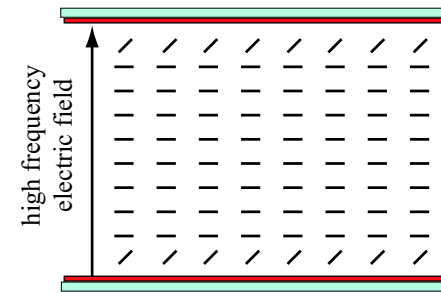
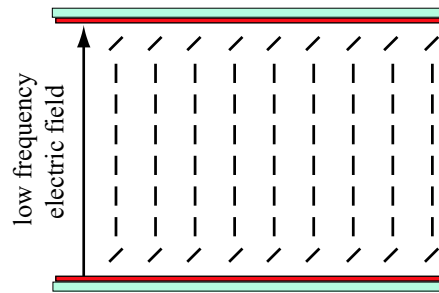
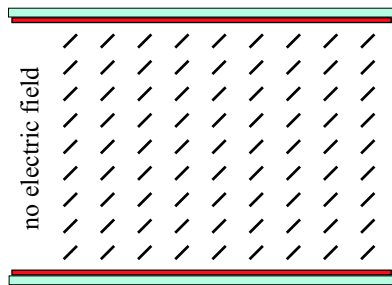


Hybrid Aligned Nematic cell



- In the right-hand case we have optimised the high frequency pulse width for switch off.

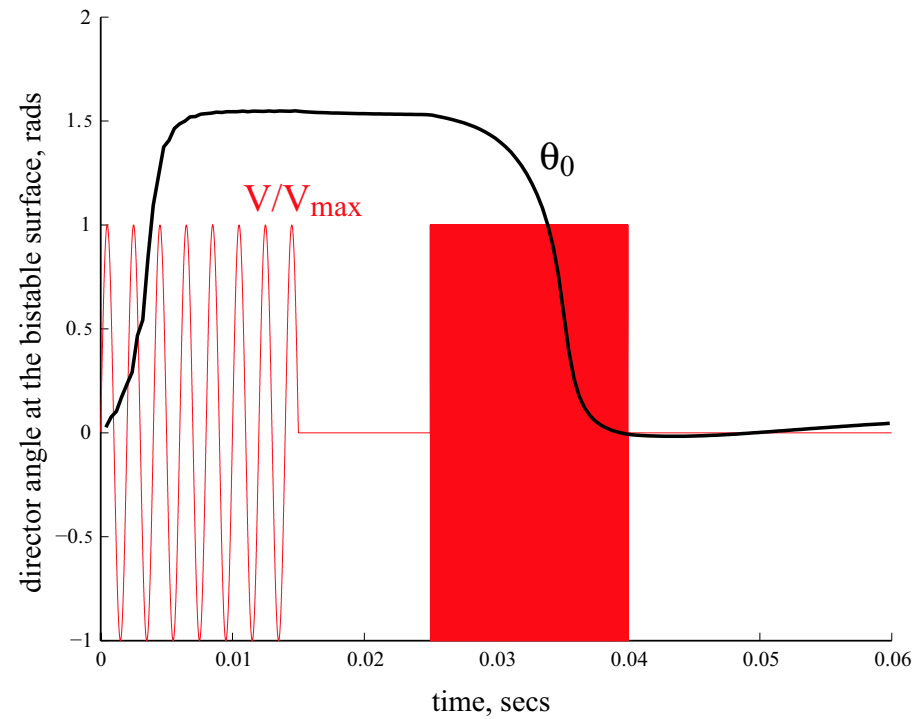
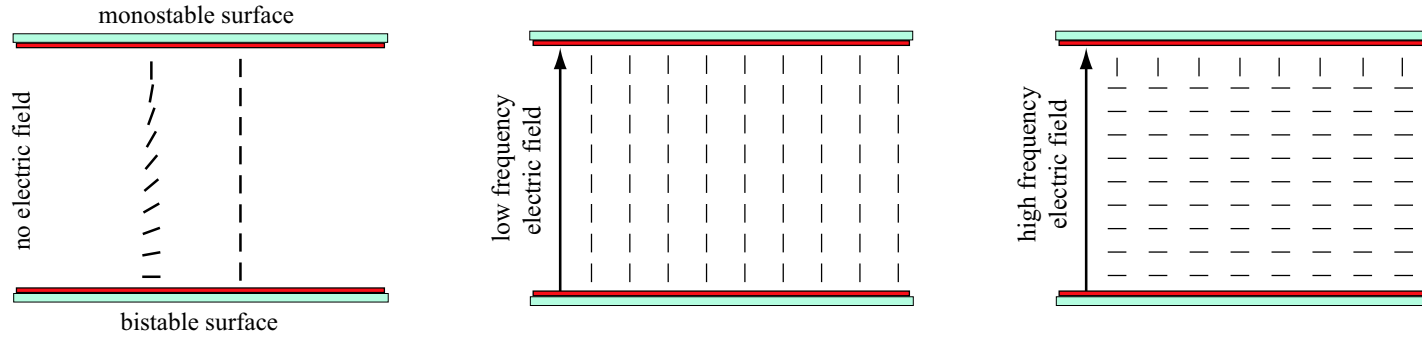
45° pretilt cell



- Maximise the electric torque on the director, optimise pulse width for switch off.

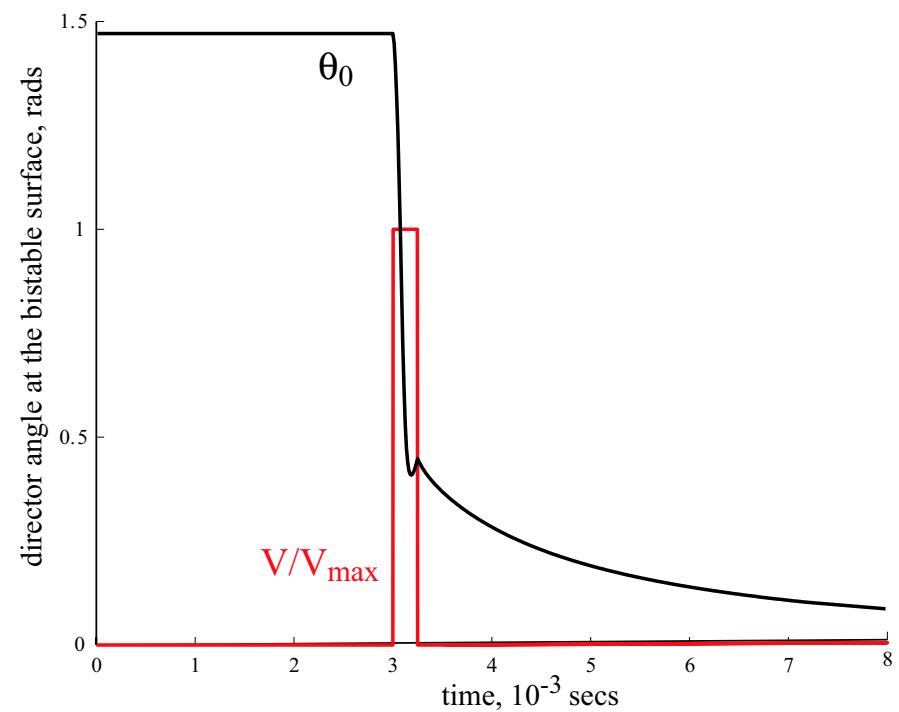
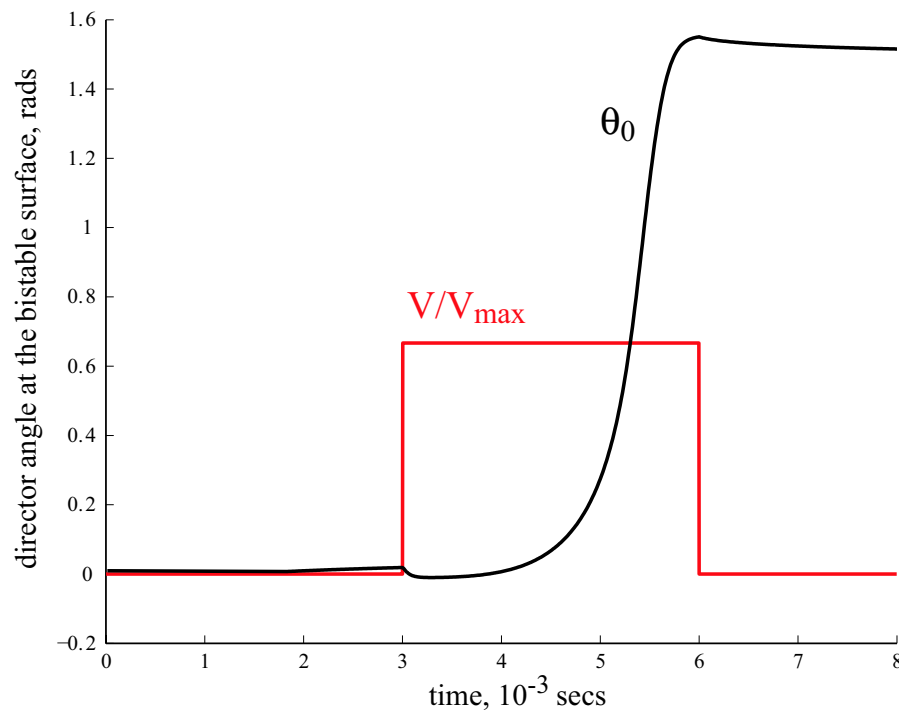
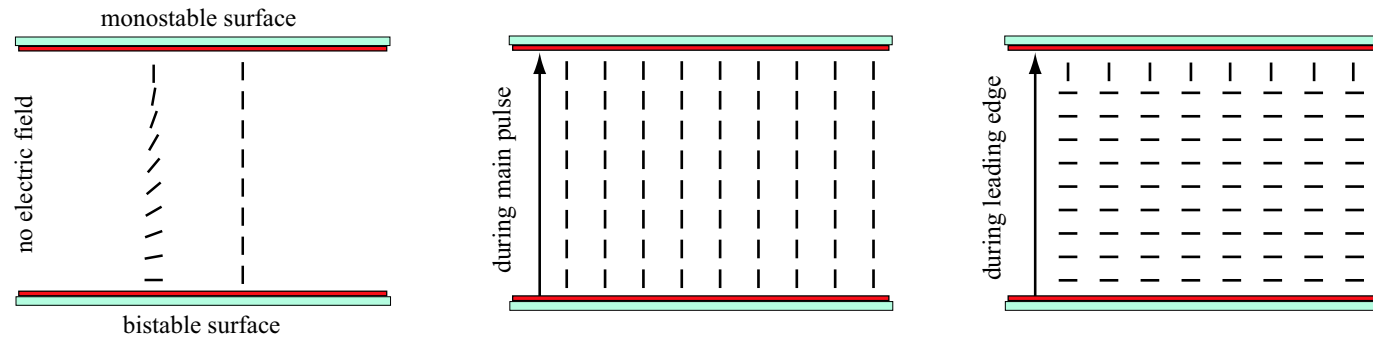
Bistable cell

- Simple bistable cell: the alignment layer at $z = 0$ allows two orientations



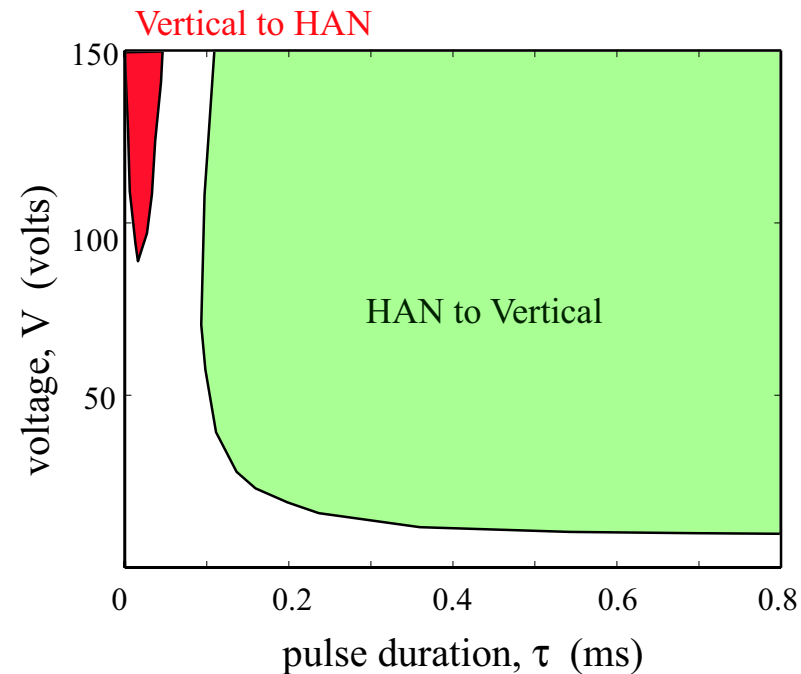
Pulsed addressing

- Constant voltage is low frequency, $\Delta\chi = \Delta\epsilon > 0$.
- Leading edge of pulse has high frequency components, $\Delta\chi = \Delta\epsilon < 0$,



Pulsed addressing: τV plot

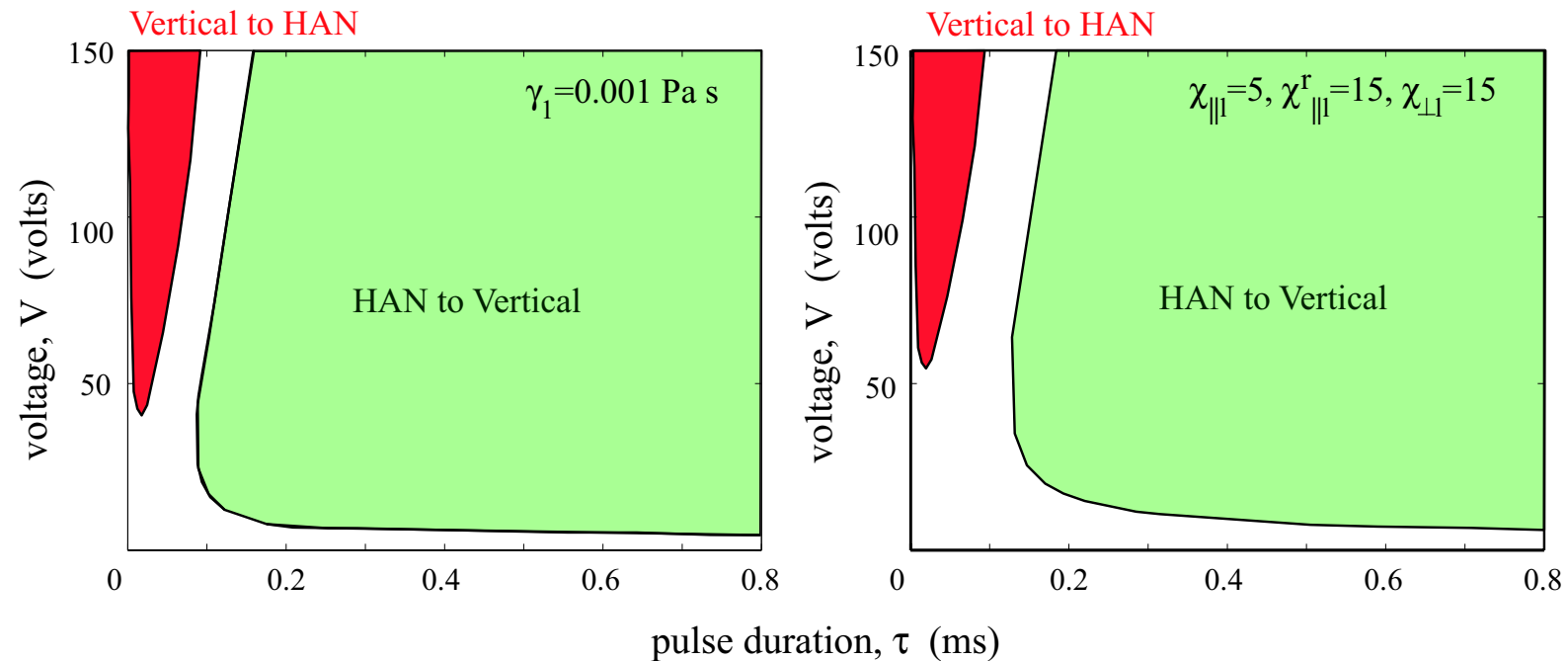
- We can apply a variety of pulses to the bistable cell to find switching regions



- Switching from the Vertical to HAN state requires very short, high voltage pulses
- Switching from the HAN to Vertical state is easier and requires sufficiently long pulses

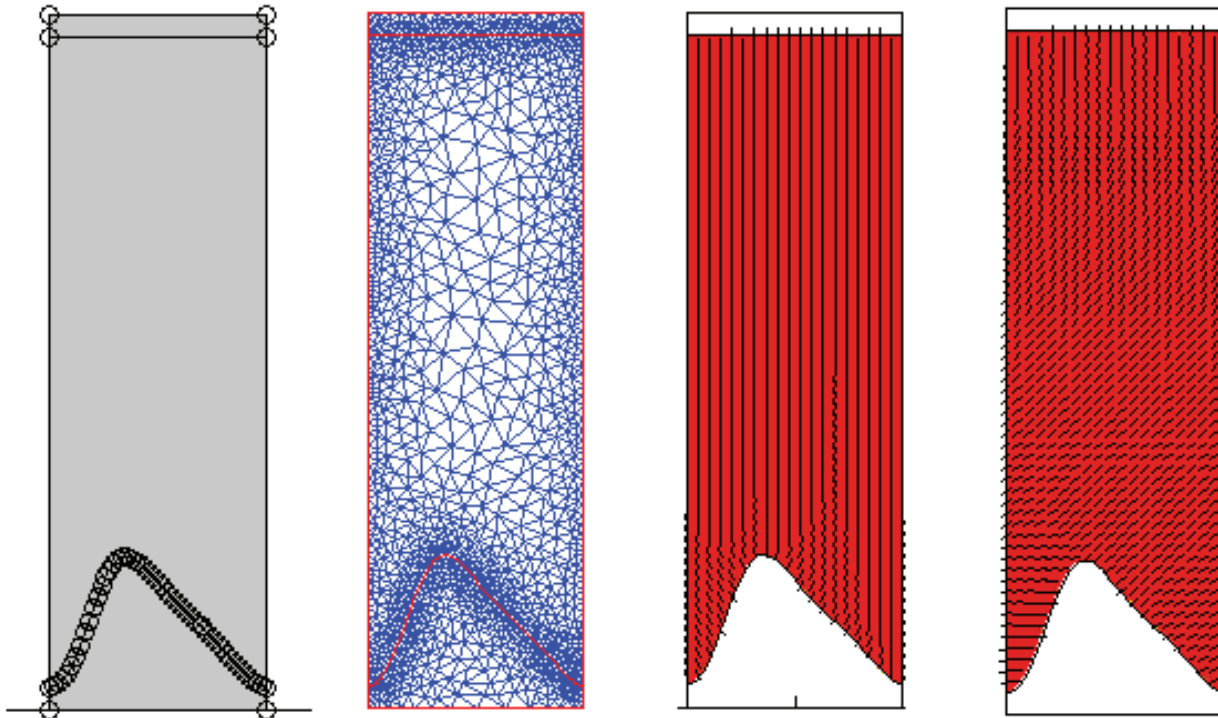
Pulsed addressing: Optimisation

- Changing the rotational viscosity and/or the susceptibilities (particularly $\chi_{\perp l}$) creates a larger Vertical to HAN switching regime.

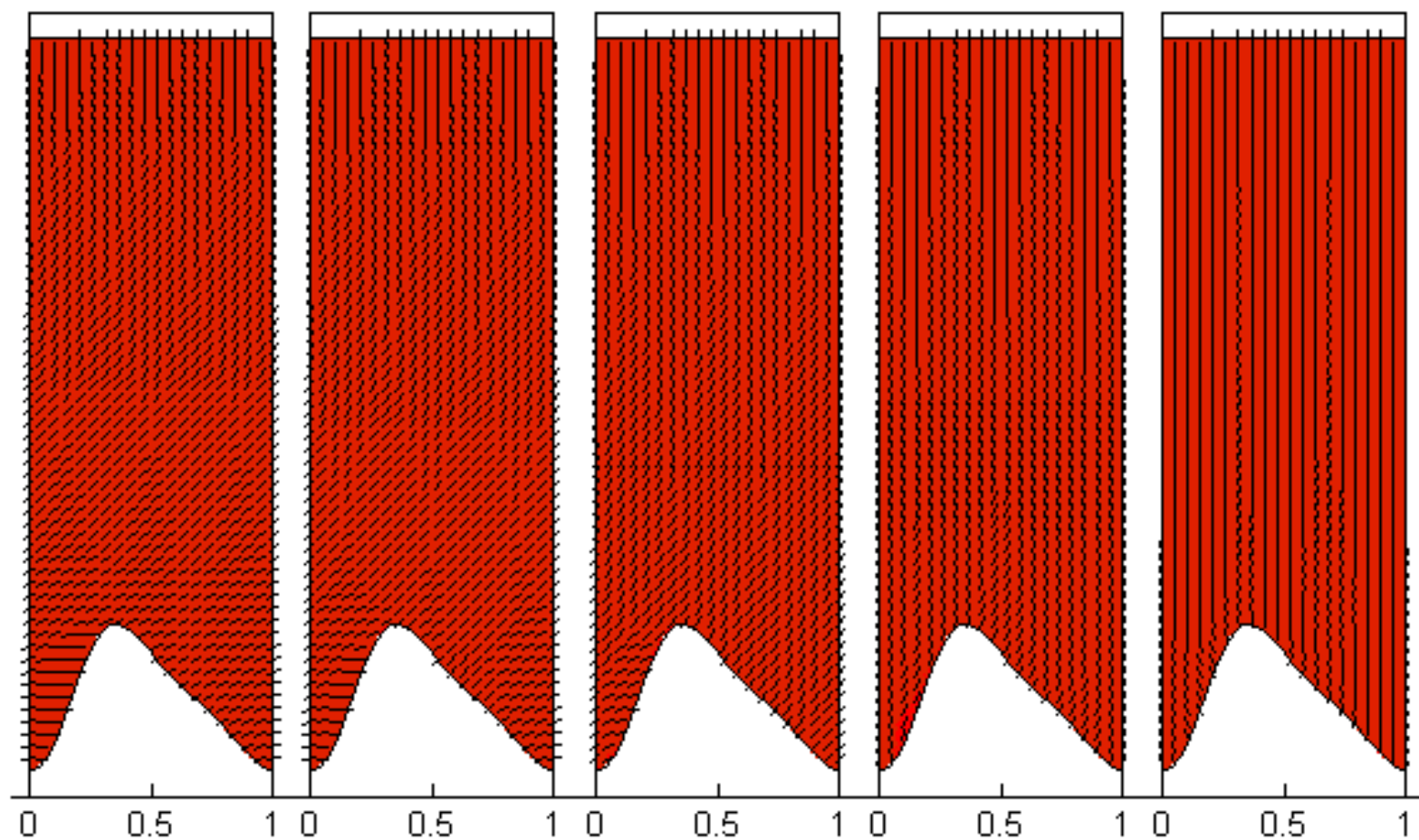


Further modelling of bistable devices

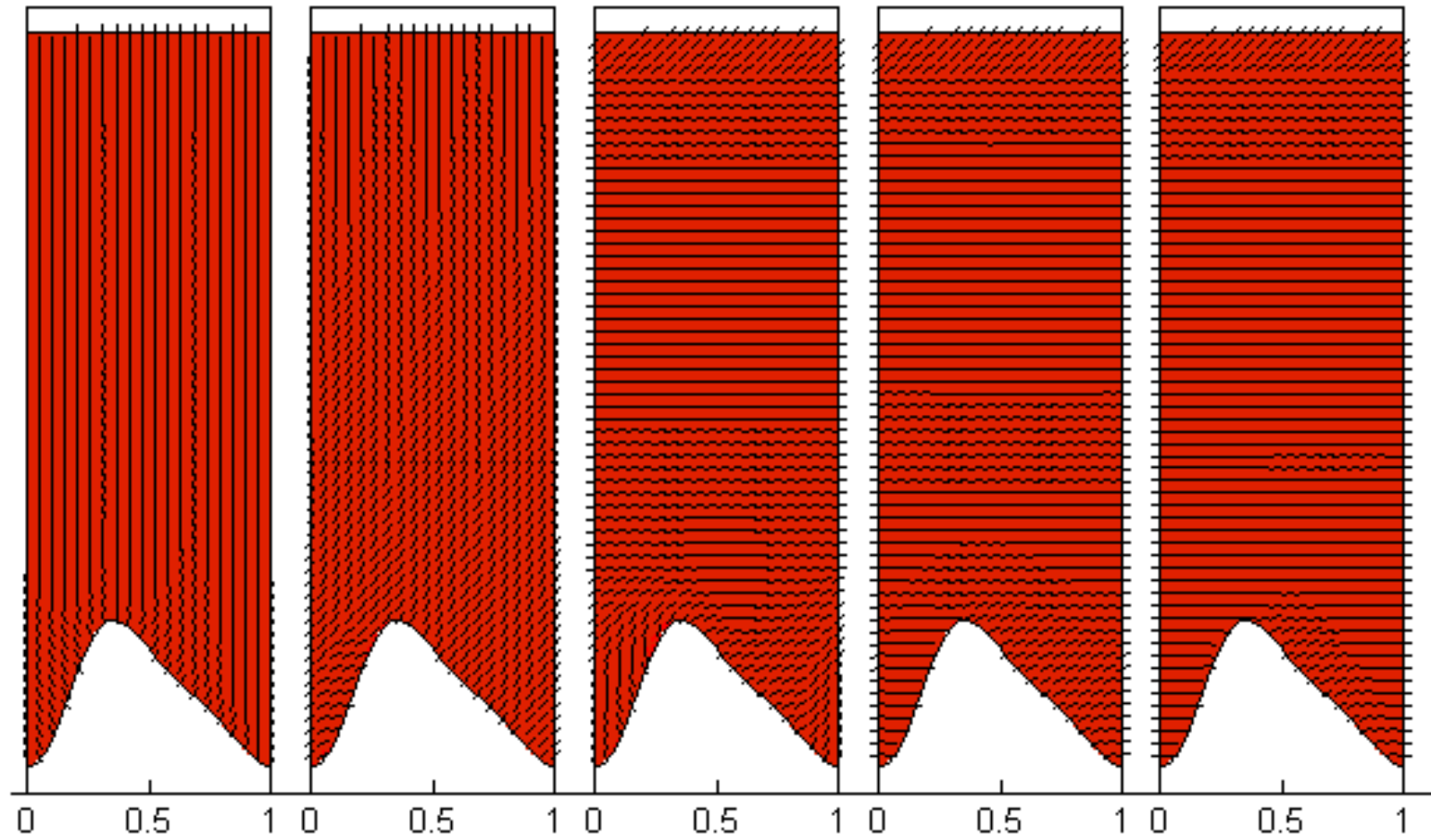
- To model a bistable device such as the Zenithally Bistable Device more accurately we need to use a 2d model.



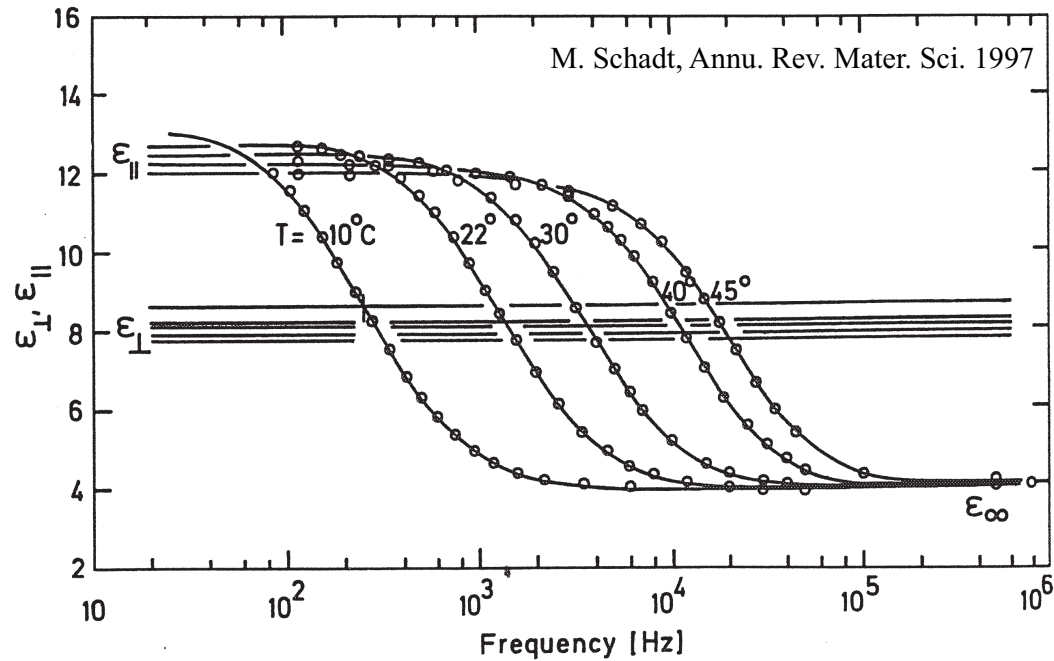
$\Delta\chi > 0$: HAN to Vertical switching



$\Delta\chi < 0$: Vertical to HAN switching



Disadvantages



- The cross over frequency, where $\Delta\chi = \chi_{\parallel} - \chi_{\perp} = 0$, is temperature dependent.
- Significant dielectric heating can occur.
- Either need optimised liquid crystal materials or a device which is temperature regulated.
- Could use driving frequencies which are far enough away from the crossover frequency.