Twist Walls in Liquid Crystal Photonic Systems

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Abstract: This paper reports on progress made in characterising twist wall stability, using computational Q-tensor models of liquid crystal systems. Twist walls are unique features that exhibit a 180^o twist of the director in a localised area. Liquid crystal anisotropy enables the optical properties of the photonic system to be programmed by manipulating an array of small electrodes. This enables photonic applications such as holographic projectors, beam steering devices and Bragg gratings [1, 2]. The stability is measured by the critical pre-tilt (PT_{crit}), where pre-tilts higher than PT_{crit} form defects rather than twist walls. Therefore the effects of the potential difference, pre-twist, anchoring strength, fill factor, structural thickness and flow on stability are studied.

1. Introduction.

Liquid crystals have unique anisotropic properties due to their cylindrical shape, meaning that the optical properties vary depending on the incident photon direction. This is utilised in twist walls by producing a switchable localised area of contrasting optical properties, in comparison to the bulk liquid crystal. Therefore a computational model [3] is used to quickly and cost effectively models the performance of experimental systems. This two dimensional finite element Matlab model implements the theory built by Ericksen-Leslie [4, 5], Qian [6] to simulate the re-orientation of liquid crystals. This model has been validated [1, 3] and effectively uses a Q-tensor method to minimise the Landau-de-Gennes free energy at each time step. The Q-tensor incorporates information on both the director and the order parameter as defined in Equation 1, where $\hat{n}$ is the principle unit director, S_1 the order parameter, S_2 the second axis biaxial order, I the identity matrix, and $\otimes$ the tensor product [2].

$$\boldsymbol{Q} = \frac{S_1}{2}(3\hat{n} \otimes \hat{n} - I) + \frac{S_2}{2}(3\hat{m} \otimes \hat{m} - I) \quad (1)$$

The photonic system contains nematic 5CB liquid crystals sandwiched between two glass plates held at (T – T* = -2K), using the recommended material coefficients in James [2] and Coles [7]. The partial twist wall above the positive electrode, illustrated in Figure 1, is enabled by applying an electric field across the photonic system. The system is as defined in Figure 1, where the left-hand side wraps around to the right-hand side in a periodic structure.

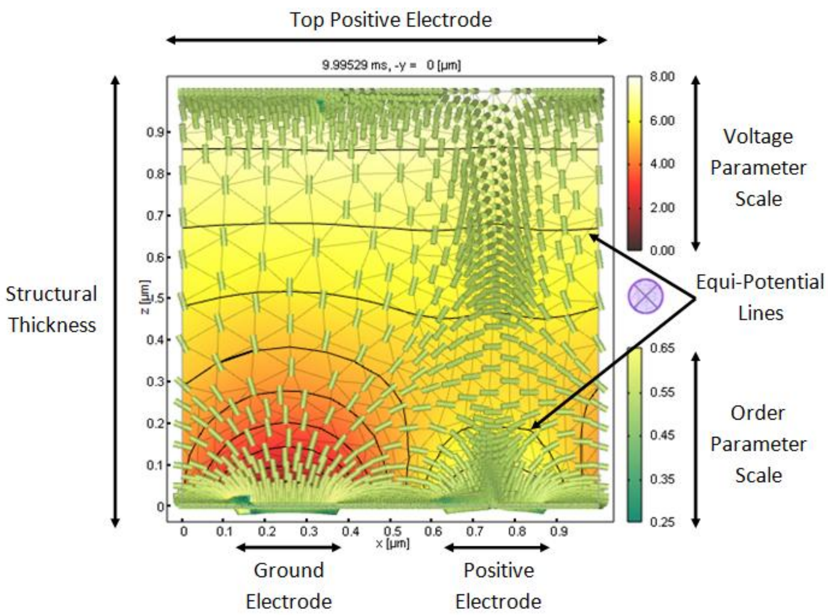

Figure 1: Steady-State Twist Wall Structure

The generalised Q-tensor program [3] is edited and streamlined by this paper, specifically to study the formation of twist walls. This includes profiling the code to identify and reduce the effects of bottlenecks, as well as removing obsolete elements and disabling functions beyond the requirements of this paper. By straddling the critical point, the critical pre-tilt is found iteratively in a systematic best estimate approach, until the desired accuracy of two significant figures is reached. The peak stability of each parameter is taken as the optimised condition and adopted for the proceeding calculations.

2. Twist Wall Formation.

The application of a potential difference across the electrodes in Figure 1 exerts an electric field induced torque on the liquid crystals, forcing the liquid crystals to re-orientate. The transient state exhibits two twist walls, a full one above the ground electrode and a partial one above the positive electrode. The full twist wall is unstable and thus it is essential to annihilate the full twist wall before it collides and destroys both twist walls and form defects. Analysis conducted in this paper identifies that voltages above 7.3V are required to induce a sweeping -½ defect illustrated in Figure 2. This sweeping defect is created by compressive forces on the liquid crystal and is essential as the translational movement upwards realigns molecules in its wake. Therefore the sweeping defect destroys the full twist wall and enables the formation of the steady-state partial twist wall as in Figure 1.

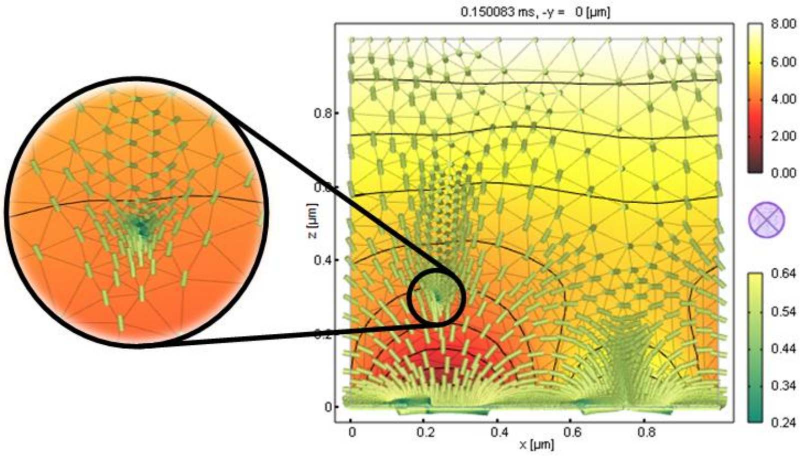

Figure 2: Transient State, Sweeping Defect at 0.15ms (8.0V, 0.27^o Pre-Tilt)

However, if the pre-tilt boundary condition exceeds PT_{crit} then before the sweeping defect is able to reach the top electrode, the full twist wall collides with the partial twist wall as shown in the transient state in Figure 3a. This annihilates both twist walls and leads to the defect steady-state in Figure 3b.

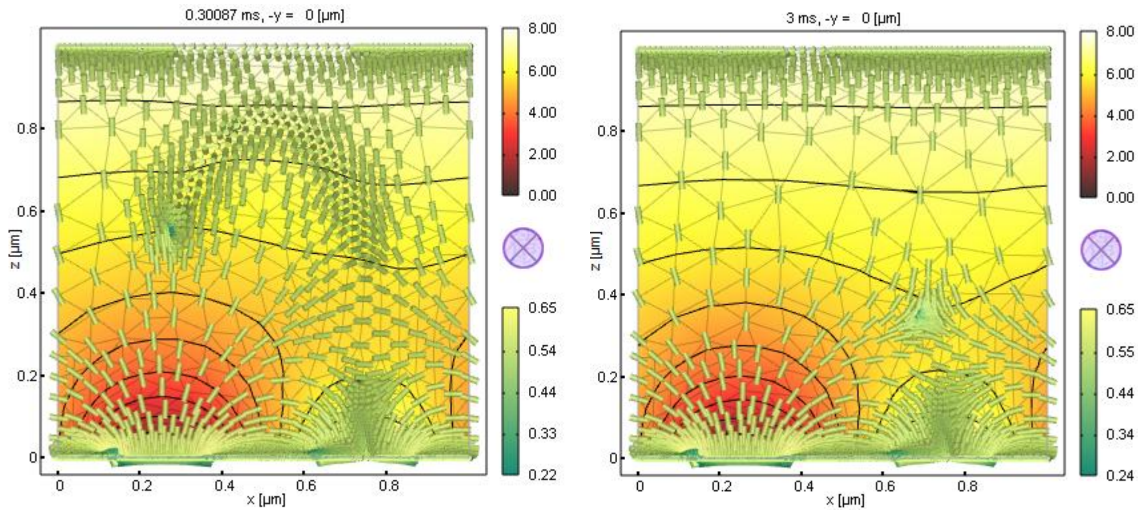

Figure 3: Defect Creation (a) 0.3ms and (b) 3ms (8.0V, 0.35^o Pre-Tilt)

3. Computational Results.

This section discusses the substantial results obtained in this paper, addressing variations in the voltage, the boundary conditions and physical structure of the system. Further analysis into twist wall formation identifies that even higher voltages exceeding the 7.3V threshold have an exponentially decaying effect detrimental to stability. Therefore an optimal value of 8.0V is selected as it exhibits high stability, whilst remaining significantly above the threshold required to induce the sweeping defect. Further tests demonstrate that removal of the electric field enables the liquid crystal system to fully recover, validating the experimental evidence of James [1]. This suggests that the force exerted by the surface anchoring boundary condition is sufficient to re-orientate the liquid crystals. The twist wall system requires 0.7ms to form a steady-state twist wall and 3.5ms for full dissipation.

A summary of the other key results are listed in Table 1, detailing the initial estimate, the optimised value and the range in which twist wall formation is possible. Twist walls only form for pre-twists greater than 35^o, with peak stability occurring at 75^o due to the length of the electrode shielding the core of the twist wall. Splay pre-tilts are proved to be twice as stable as planar pre-tilts as it enables greater system symmetry in the liquid crystal bulk. The effect of strong/weak anchoring is found to be negligible, with the strong case exhibiting slightly enhanced recovery characteristics. A phenomenon of critical shielding occurs at fill factors greater than 67% as the twist wall is completely shielded, preventing the formation of the -½ sweeping defect. Otherwise a linear positive correlation is observed where higher fill factors exhibit higher stability and thus a fill factor of 60% is selected. The analysis also suggests that a 0.1μm reduction in structural thickness increases stability by 65%, where the 8.0V potential difference is too weak to induce the sweeping defect in thicknesses above 1.2μm. The flow is highly dependent on temperature, thus the no flow case represents the worst case scenario as liquid crystal flow enhances stability by making it easier for the sweeping defect to move upwards.

Parameter Condition	Initial	Optimal	Range
Potential Difference (V)	10.0V	8.0V	>7.3V
Pre-Twist Type (^{o})	Planar 85^o	Planar 75^o	Planar 35^o to 90^o
Pre-Tilt	Splay	Splay	Planar or Splay
Surface Anchoring	Strong	Strong	Weak or Strong
Fill Factor (%)	50	60	5 to 67
Structural Thickness (μm)	1.0	0.9	<1.2
Flow	No	Yes	Optional

Table 1: Initial, Optimal and Range of the Parameter Conditions

Implementing the optimal parameter conditions in Table 1 for the pre-twist case, and contrasting it with the initial settings, leads to the results illustrated in Figure 4. The results show that twist wall stability is increased for all pre-twists, with peak stability improving by 55%. This is achieved by differentiating the curve fit to find the point of peak stability, which also identifies a slight shift to the left. This verifies the assumption that parameters are independent or only loosely dependent.

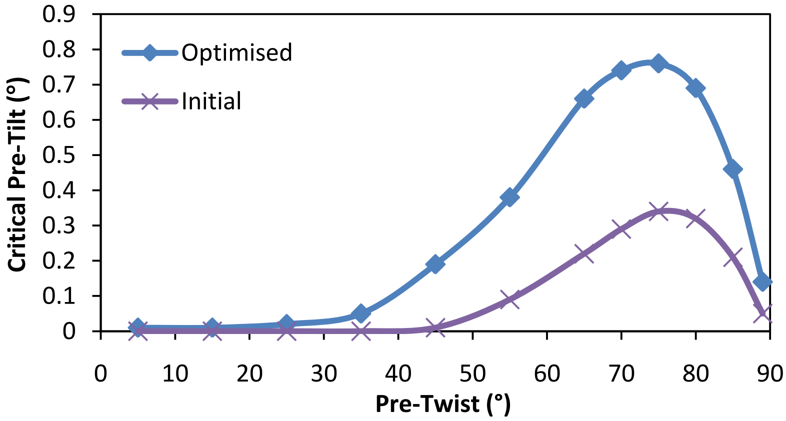

Figure 4: Pre-Twist Stability Variation

4. Conclusions.

The results indicate that only the single partial twist wall above the ground electrode is possible at steady-state, though semi-stable dual and full twist walls may also be observed. The stability of the photonic liquid crystal system is a race between whether a fully swept defect or twist wall collision occurs first. The -½ defect induced at voltages greater than 7.3V is essential for twist wall formation, as it realigns the liquid crystal molecules in its wake when sweeping upwards, destroying the unstable full twist wall. The liquid crystal system has also demonstrated full theoretical recovery, making it ideal for programmable applications.

Peak stability is demonstrated at 75^o pre-twist due to the shielding effects of the electrode length. This reinforces the observations of critical shielding in systems with fill factors greater than 67%, which entirely shields the centre of the twist wall from the positive ground electrode and thus does not induce the critical sweeping defect. Though both pre-tilt types are possible, the splay case exhibits significantly greater stability than the planar case. Stability is shown to be independent of surface anchoring strength, though exhibiting high sensitivity to the structural thickness. Liquid crystal flow is demonstrated to enhance stability by making it easier for the defect to translate upwards.

The recommended optimised conditions discovered in this paper for twist wall creation are 8.0V, 75^o planar pre-twist, splay pre-tilts, strong anchoring, 60% fill factor and 0.9µm structural thickness. These optimised parameters demonstrate increased stability across all variables, and typically demonstrate a 55% improvement in peak stability from the initial pre-optimised conditions.

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