Capacitive Based Liquid Crystal Chemical and Biological Sensors

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Abstract—**This paper demonstrates the principle of capacitive sensing in liquid crystal (LC) based sensors with potential applications to chemical and biological systems. The theory for tracking the average molecular deformation partially disorder LC film via capacitive sensing is investigated. Three capacitance measurements are required to track the average molecular orientation as well as the degree of disorder in the LC film. Sensors' outputs are digitized by involving capacitance to digital converter to be applied to computerized applications. Both the experimental and calculated capacitances of a selected sensor structure are presented.**

Fig. 1.   Rapid and sensitive detection of organophosphonates [3]

I. INTRODUCTION

Liquid crystals (LCs) have recently been demonstrated to be excellent candidates for low cost, portable, highly selective chemical and biological sensors [1]-[3]. In these sensors, the molecular alignment of the liquid crystal is altered by the presence of targeted chemical or biological agents. Surface driven orientational changes in LC films have proven to be highly effective in amplifying the presence of targeted analytes in chemical and biological sensors. In all these sensors, optical transduction has been used to sense the deformations within the LC material. An example of the visual change is shown in Fig. 1 in which the presence of organophosphonates is detected.

In a previous work [4], the authors presented a capacitive transduction technique for ordered LC systems that offered significant advantages over the optical techniques. For example, the ability to identify and track the deformation rather than simply sensing an LC distortion. The authors theoretically proved and experimentally verified that two capacitive measurements can uniquely track changes of the molecular orientation in an ordered LC film. Although the effort in [4] has been demonstrated in fully ordered systems, LC films in practical sensors are partially disordered. The innovation of this paper is to extend the capacitive transduction method to simulate inhomogeneous, partially disordered and highly anisotropic LC films. These techniques will lead to more practical and enhanced LC sensor systems. The theory and experiments are expanded to handle partially disordered LC films. In this case, three capacitance measurements are required to track the director axis and the order parameter.
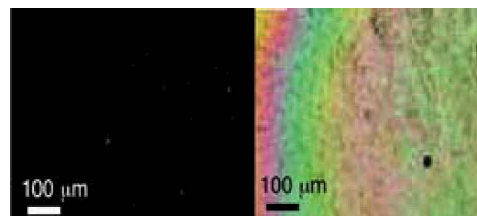
II. CAPACITIVE SENSING IN LIQUID CRYSTALS

The capacitive sensing in LC based sensors exhibits a change in capacitance in response to a change in the molecular alignment in the LC film. In these sensors, the molecular alignment in an LC film is altered in response to some environmental condition. For most chemical and biological sensors, the orientational behavior of LCs near surfaces is exploited. A homeotropic alignment will change to homogeneous as was demonstrated by Abbott and Shah [3] in detecting part-per-billion concentration of dimethylmethylphosphonate (DMMP). Another example is when a homogeneous alignment at a given angle will rotate to a homogeneous alignment at a different angle as shown in [3]. Due to the collective behavior of molecules forming LCs, a change in the structure at the surface caused by the binding of a chemical or biological agent is amplified into a significant change in the average molecular alignment of the LC film.

The objective of this paper is to provide insight into the molecular behavior inside the LC film and to track the average molecular distortion (the director axis) and the degree of the orientational order (the order parameter) in partially disordered LC based sensors via capacitive transduction. Moreover, the LC film will be assumed to be anisotropic and inhomogeneous over the area of interest. Therefore, the film can be represented as a uniaxial crystal that exhibits two electrical permittivities, a parallel permittivity, $\epsilon_\parallel$, for the electric field traveling in parallel with the long molecule axis and a perpendicular permittivity, $\epsilon_\perp$, for the electric field traveling in perpendicular with the long molecule axis. In the molecular principal coordinate system, the permittivity tensor, ϵ_m, is given by [5]

$$\epsilon_m = \begin{bmatrix} \epsilon_\perp & 0 & 0 \\ 0 & \epsilon_\perp & 0 \\ 0 & 0 & \epsilon_\parallel \end{bmatrix}. \qquad (1)$$

The long molecule axis is described by Euler's angles θ_r and ϕ_r. In general, these angles are treated as random variables. The orientation of the average molecular orientation is called the director axis which is defined by the zenithal angle, θ, which lies between the director axis and the z-axis and the azimuthal angle, ϕ, which lies between the x-axis and the projection of the director axis onto the x-y plane. Let the director axis be represented by $\vec{n}$, without loss of generality, the director axis has a unit length, i.e. $|\vec{n}| = 1$. The vector $\vec{n}$ can be expressed in Cartesian coordinates in terms of the standard Euler's angles, θ and ϕ, as [6]

$$\vec{n} = \sin\theta\cos\phi\,\hat{x} + \sin\theta\sin\phi\,\hat{y} + \cos\theta\,\hat{z}. \qquad (2)$$

The degree of the molecular disorder in an LC film is described by the order parameter which is given by [7]

$$S = 0.5 < 3\cos^2\theta_r - 1 >, \qquad (3)$$

where the triangle brackets represent the statistical average. The order parameter is equal to one when all molecules lie parallel to the director axis, i.e. $\theta_r = 0$ (perfect uniaxial crystal) and zero when the orientation of the molecules is completely random [7].

The effective permittivity tensor in Cartesian coordinates is described in terms of θ and ϕ and S. Therefore, the capacitances are also depend on these angles. As a result, the measurement of the capacitance will lead to the director axis orientation and the order parameter.

III. SENSOR STRUCTURE

The interdigitated electrodes configuration is a recommended structure for tracking the average director axis of an LC film via capacitive sensing. A possible electrode design consists of two perpendicular interdigital cells as shown in Fig. 2. These interdigitated electrodes are patterned on one substrate where a continuous electrode is on the other substrate. An LC film of thickness d is sandwiched between these substrates as shown in Fig. 3. In Fig. 2, a top view of two perpendicular interdigitated cells in x-y plane is shown while Fig. 3 shows cross section of one unit cell of the sensor in the x-z plane.

By applying different electrical potentials to the interdigitated electrodes, two fringing capacitances can be measured, namely C_{F1} and C_{F2}. The capacitance C_{F1} is measured between V_1 and V_c where C_{F2} is measured between V_2 and V_c as shown in Fig. 2. On the other hand, the capacitance associated with the transverse electric field shown in Fig. 3 is called the transverse capacitance and denoted by C_T. The transverse capacitance can be measured between the interdigitated electrodes and the top electrode. It is important to notice
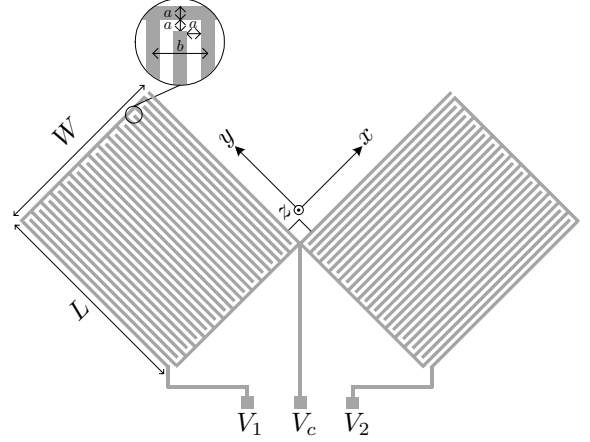

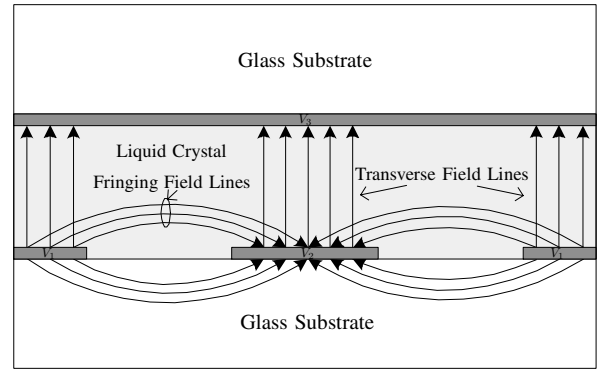Fig. 2. Top view of the candidate LC sensor

Fig. 3. Cross Section of one cell of the candidate LC sensor

that the potentials used to measure the capacitance in this sensor should not exceed the Freeddericksz transition strength or the LC molecules will rotate as function of the potential [8].

Results will show later that the tranverse capacitance depends on θ and S where the fringing capacitance depends on θ, ϕ and S. Measuring three orthogonal capacitances (two fringing and one transverse) lead to the zenithal angle, θ, the azimuthal angle, ϕ, and the order parameter, S.

IV. CAPACITANCE CALCULATION

Although some techniques are used to derive closed form for the interdigitated structure capacitance associated with homogenous and isotropic material such as conformal mapping [9], no analytical form exists to calculate this capacitance in the presence of anisotropic material. In this section, a numerical method will be used to calculate the capacitances of the interdigital structure in the presence of LC material. Since the LC film is assumed to be anisotropic, the electric field in LC film satisfies the Maxwell's equation [5]

$$\nabla \cdot (\bar{\epsilon}\vec{E}) = 0, \qquad (4)$$

where $\bar{\epsilon}$ is the average permittivity tensor and $\vec{E}$ is the electric field vector, both in Cartesian coordinate system. The

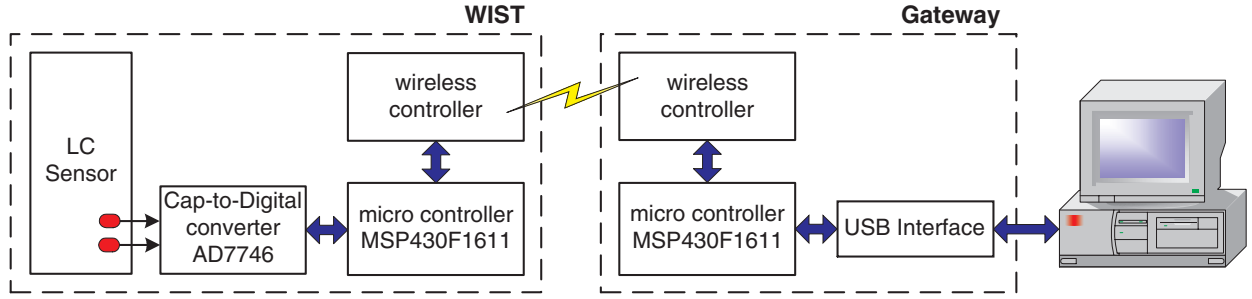Fig. 4. Block diagram of the wireless sensing system

statistical average of the permittivity tensor is given by

$$\bar{\epsilon} = \frac{2\epsilon_\perp + \epsilon_{||}}{3}\mathbf{I} + \Delta\epsilon\,\mathbf{Q} \tag{5}$$

where $\mathbf{I}$ is a 3×3 identity matrix, and $\mathbf{Q}$ is a tensor given by

$$S\begin{bmatrix} \sin^2\theta\cos^2\phi - \frac{1}{3} & \sin^2\theta\sin\phi\cos\phi & \sin\theta\cos\theta\cos\phi \\ \sin^2\theta\sin\phi\cos\phi & \sin^2\theta\sin^2\phi - \frac{1}{3} & \sin\theta\cos\theta\sin\phi \\ \sin\theta\cos\theta\cos\phi & \sin\theta\cos\theta\sin\phi & \cos^2\theta - \frac{1}{3} \end{bmatrix}. \tag{6}$$

The permittivity tensor, $\bar{\epsilon}$, depends on the LC deformation parameters; θ, ϕ and S. The capacitances between the electrodes are calculated as follows

- Consider $\bar{\epsilon}$ from (5) and (6)
- Solve (4) for $\vec{E}$ by applying finite difference method
- Calculate the charge per unit length, Q, by applying Gauss's law to a closed path, ℓ, enclosing the electrode where

$$Q = \oint_\ell \bar{\epsilon}\vec{E} \cdot d\vec{l} \tag{7}$$

- The capacitance per unit length between any two electrodes is given by

$$C = \frac{Q}{V_d}, \tag{8}$$

where V_d is the potential difference between the two electrodes.

V. CIRCUIT IMPLEMENTATION

Current generation of MEMS and nano sensors requires precise capacitance measurements in noisy environment. We designed a portable wireless sensor platform for field deployment. The platform is called Wireless Sensor Transducer (WIST). The system measures single or differential capacitance of the physical sensing device, processes data, and sends the measurements wirelessly to a gateway system. The system has three major components, a dedicated capacitance-to-digital converter, an ultra low power microcontroller, and a wireless controller as represented in Fig. 4.

The capacitance to digital converter is AD7746 from Analog Devices. The single-chip controller has several features that were very important for our target applications:

- Very high resolution (24 bit)
- Single or differential capacitance measurement
- Common-mode capacitance measurement up to 17 pF
- Accuracy: 4 fF
- Linearity: 0.01%
- On-chip temperature sensor
- I2C compatible 2-wire serial interface
- 2.7 V to 5.25 V single-supply operation
- Very low power (active 4.25 mW, idle 10 μW)
- Simultaneous 50 and 60 Hz rejection

We use Texas Instruments microcontroller MSP430F1611. The MSP430 family was chosen because of ultra low power consumption, while the F1611 was chosen because of a variety of communication capabilities two USARTs that can be configured as asynchronous or synchronous serial controllers. The device features 10 KB of RAM and 48 KB of flash memory, which is the higher amount of RAM in the MSP430 family. In addition, F1611 features a fast interrupt wake-up time and a DMA controller which allows data transfers without waking up the processor, which further improves power efficiency of our application. These characteristics make F1611 a perfect application development microcontroller.

Wireless communication is controlled by 2.4 GHz wireless controller 24L01 from Nordic. This is an intelligent wireless controller with high bandwidth (1 Mbps), medium range (~ 50 m), and ultra low power consumption. This enables communication of several sensors with wireless gateway. Wireless gateway communicates with a laptop or a workstation.

VI. SIMULATION AND EXPERIMENTAL RESULTS

In this section, simulation and experimental results are presented to provide insight into capacitive transduction for the electrode design shown in Fig. 2. The sensor parameters and the LC material used in the simulation and experimental parts are shown in Table I.

TABLE I
SIMULATION AND EXPERIMENTAL SENSOR PARAMETERS

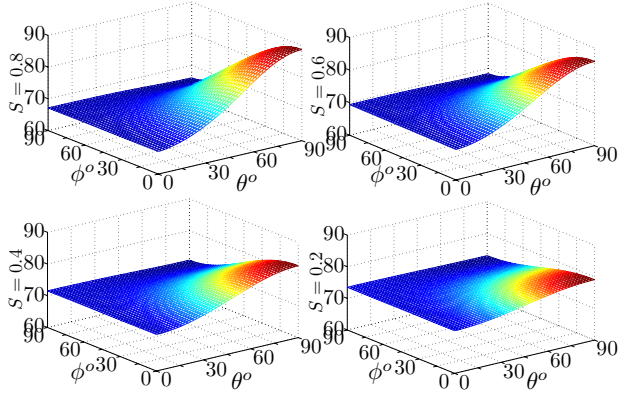| Parameter	LC	L	W	a	b	d
Unit		mm	mm	μm	μm	μm
Simulation	5CB	4	4	4	16	4
Experimental	BL006	5.5	5	10	40	51

Fig. 5. Fringing capacitance, C_{F1}, in pF as a function of θ and ϕ.
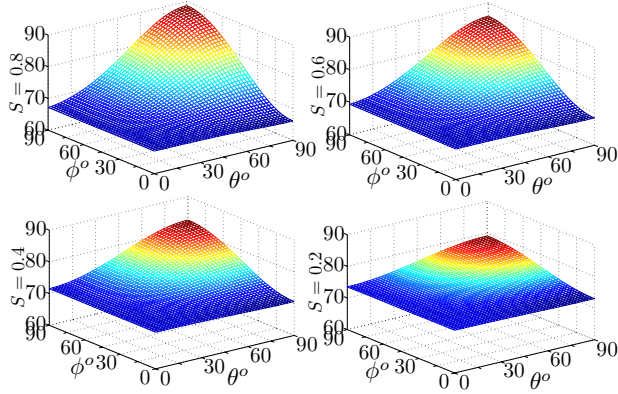
Fig. 6. Fringing capacitance, C_{F2}, in pF as a function of θ and ϕ.

Fig. 7. Transverse capacitance, C_T, in pF as a function of θ.
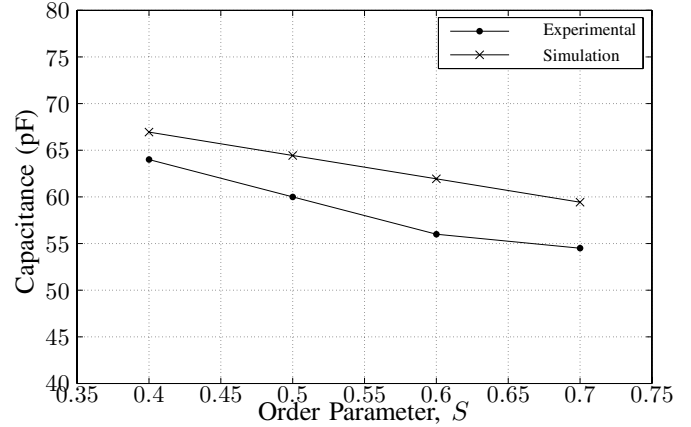
Fig. 8. Capacitance, in pF, versus S with initial alignment at $\theta = \phi = 90^0$

The calculated fringing capacitances C_{F1} and C_{F2} as functions of θ and ϕ at $S = 0.2, 0.4, 0.6$ and 0.8 are shown in Figs. 5 and 6, respectively. The calculated transverse capacitance as a function of θ at different values of S is shown in Fig. 7. A prior knowledge of how the orientation of the LC molecules will likely reorient in response to some environmental stimulus is critical to optimizing the performance of the sensor. The electrode structure and the initial state of orientation impact the sensitivity. The behavior of the sensor was investigated experimentally in the presence of BL006 LC film and the parameters given in Table I. The molecules were aligned initially to behave as a homogenous texture with $\theta = \phi = 90^o$. The sample was heated so a reduction in the degree of order is occured. The capacitance was measured at different temperature values and then the order parameter was extracted from the temperature curve. Some values of the capacitance as a function of S are given in Fig. 8.

VII. SUMMARY

The method of capacitive transduction for LC-based sensors has been presented and tested. Sensors with interdigitated electrodes can be used to track the director axis of a partially disordered nematic LC film. Three capacitance measurements are required to track the LC molecular deformation.
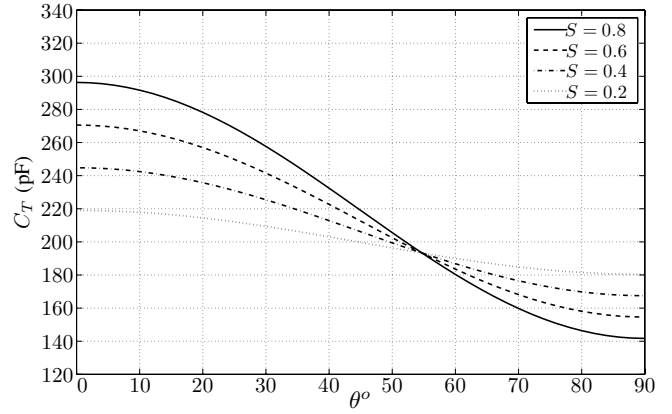
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