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Numerical Determination of Thermal-Diffusivity Coefficients of Some Nematic Liquid Crystals *in Situ*

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Abstract In this study, a new experimental study has been implemented to determine the thermal-diffusivity parameters of industrial nematic liquid crystals, 4-pentyl-4′-cyanobiphenyl (5CB) and 4′-octyl-4-cyanobiphenyl (8CB), both numerically by using the finite difference method (FDM) for forward solutions and experimentally by measuring the temperature variation with time and position. The most important parts of this experimental study are the heating system and the liquid crystal cell, which were constructed in-house to determine the temperatures of the materials in situ. Four different positions for local measurements have been studied, and the optimum graph of this variation has been determined. The experimental and theoretical results of this study are consistent with previous measurements performed by means of a conventional thermal technique.

Keywords Finite difference method · Liquid crystals · Thermal diffusivity

1 Introduction

Liquid crystals are materials that show characteristics that are unique electric, optical, and thermal properties. These properties of the liquid crystals are generally determined by the rigid core of the molecules. This is because the core generally contains two or more benzene rings that have a high density of delocalized electrons. The core is therefore highly polarizable and the dominant part of the molecule in terms of optical, thermal, and dielectric properties. The orientational order of liquid crystals combined with their molecular anisotropy leads to anisotropic physical properties, as for an anisotropic crystalline solid. In the same way that the optical properties of the liquid

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crystals are anisotropic, so too are the dielectric properties: the polarization induced by an applied electric field depends on the direction of the field.

Transport properties of nematic liquid crystals have been studied extensively, because the thermal conductivity of the nematic phase is temperature dependent [1]. In recent years, it was recognized that convection within a heated nematic liquid crystal provides an interesting, rich system for the study of pattern formation under nonequilibrium conditions. After a number of early qualitative investigations, quantitative theoretical predictions and experimental measurements became available. Thermal parameters that change with variations of the molecular orientation in liquid crystals led to further studies of these widely used technological materials. Of the various photothermal methods, photoacoustic and photopyroelectric techniques are commonly used for thermal characterization as well as for phase-transition studies of liquid crystals. The thermal diffusivity of liquid crystals is extremely important not only simply because it is a unique thermophysical parameter but also for the accurate determination of the thermal conductivity or specific heat capacity. By knowing these parameters, the evaluation of the density of liquid crystals can be easily carried out. A combination of the present technique allows the complete thermal characterization of the liquid crystals and other non-absorbent liquids [2].

Thermal wave physics and related photothermal effects emerged as an effective research and analytical tool for the characterization of thermal, transport, and optical properties of materials in different states. Based on the results obtained from these studies, the technological use of liquid crystals has increased [3,4]. Liquid crystal displays (LCDs) for calculators, computers, watches, and thermometers are common examples of liquid-crystal uses in various applications. Especially, considerable effort was applied in the synthesis and characterization of liquid crystals due to their wide applicability in the photonics industry. Today, liquid crystals are widely used in the electrical device market and in LCD technology centers [5–8].

In this study, we attempted to determine the thermal-diffusivity parameters of liquid crystals 5CB and 8CB both numerically by using the finite difference method (FDM) for forward solutions and experimentally by measuring the variation in temperature with time and position. The most important parts of this experimental study were the measured temperature data of the materials *in situ*. The thermal data were obtained for random orientation due to the properties of molecular anisotropy. In a further study, we plan to determine the thermal-diffusivity parameters for aligned molecular anisotropy, so that the results for random orientation and aligned molecular anisotropy of the liquid crystal materials can be compared.

2 Theory and Numerical Model

The most direct method of determining the thermal conductivity consists of a measurement of the temperature difference and application of the explicit finite difference method (FDM). This method is used for estimating the functional value of unknown points. It is represented with thermal differences at the spatial temperature nodes and is required for several numerical procedures of calculations [9–13].

It is well known that the diffusivity equation of materials with spatial-time correlation, which is represented by the thermal conductivity, is expressed as follows:

$$\frac{\partial^2 T}{\partial x^2} = \frac{1}{\alpha}\frac{\partial T}{\partial t} \tag{1}$$

where α is the thermal-diffusivity coefficient. This equation can be arranged in a finite difference form using the explicit method as follows:

$$\frac{\partial^2 T}{\partial x^2} = \frac{T^i_{m+1} + T^i_{m-1} - 2T^i_m}{(\Delta x)^2} \tag{2}$$

$$\frac{\partial T}{\partial t} = \frac{T^{i+1}_m - T^i_m}{\Delta t} \tag{3}$$

By substituting Eqs. 2 and 3 into Eq. 1,

$$\frac{T^i_{m+1} + T^i_{m-1} - 2T^i_m}{(\Delta x)^2} = \frac{1}{\alpha}\frac{T^{i+1}_m - T^i_m}{\Delta t} \tag{4}$$

where T^{i+1}_m is the temperature of the mth node point at time $t + \Delta t$.

The derivative of function $T(x)$ at the point X_m may be written as

$$\left(\frac{\mathrm{d}T}{\mathrm{d}x}\right)_{x_m+\Delta x} = \lim_{\Delta x \to 0} \frac{T_{x_m+\Delta x} - T_x}{\Delta x} \cong \frac{T_{m+1} - T_m}{\Delta x} \tag{5}$$

This function represents the first derivative of the forward difference form. Similarly, the backward derivative of function $T(x)$ at the point X_m becomes

$$\left(\frac{\mathrm{d}T}{\mathrm{d}x}\right)_{x_m-\Delta x} = \lim_{\Delta x \to 0} \frac{T_{x_m} - T_{x_m-\Delta x}}{\Delta x} \cong \frac{T_m - T_{m-1}}{\Delta x} \tag{6}$$

By substituting Eqs. 5 and 6, we obtained a new distribution form of temperature as follows:

$$\left(\frac{\mathrm{d}T}{\mathrm{d}x}\right)_{x_m} = \frac{T_{m+1} - T_{m-1}}{2\Delta x} \tag{7}$$

This expression is the central form of the derivative of function $T(x)$ at the point X_m.

3 Experimental Design

In this study, thermal-diffusivity coefficients of commercially available 4-pentyl-4′ cyanobiphenyl (5CB) and 4′-octyl-4-cyanobiphenyl (8CB) liquid crystals were investigated for the nematic phase with random molecular orientation. The liquid crystals are convenient to work with since they show a nematic phase at room temperature. In

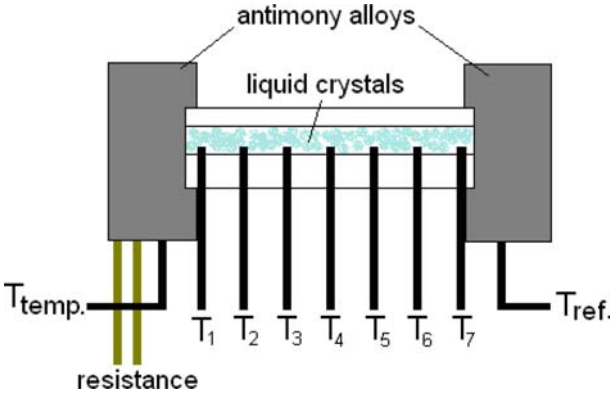

Fig. 1 Representative illustration of thermal unit system and liquid crystal cell

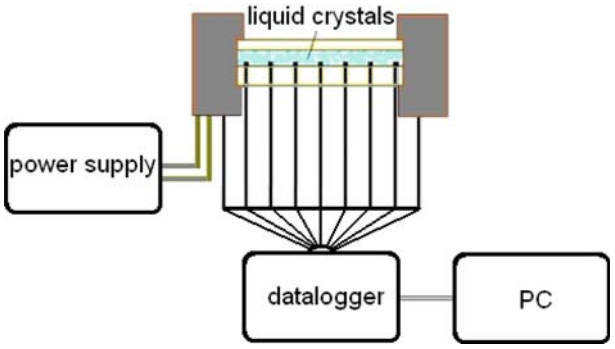

Fig. 2 Experimental measuring system

the experiment, thermocouples were placed at four different locations in the crystal to determine the spatial temperature variation as seen in Fig. 1, in situ. The obtained data were graphed, and through curve-fitting techniques, an optimum equation was found, which was then numerically solved using the forward finite difference method in order to find the thermal-diffusivity coefficients of the liquid-crystal samples studied.

Temperatures at different node points were measured by thermocouple probes attached to a Consort Model T851 datalogger as seen in Fig. 2. Measurement intervals were determined between 25 °C and 32 °C for 5CB and between 35 °C and 40 °C for 8CB. A temperature rate of $0.1\,^{\circ}\mathrm{C}\cdot\mathrm{s}^{-1}$ was employed in all measurements.

4 Results and Discussion

In this study, the thermal diffusivity of the nematic liquid crystals 5CB and 8CB was investigated for random molecular orientation and *in situ* cell conditions. For the 5CB sample, the thermal diffusivity was measured in the temperature range from 25 °C to 32 °C and varied between $0.95\times10^{-7}\,\mathrm{m}^2\cdot\mathrm{s}^{-1}$ and $1.15\times10^{-7}\,\mathrm{m}^2\cdot\mathrm{s}^{-1}$ as seen in Fig. 3. Similarly, the thermal diffusivity of the 8CB sample was measured in the

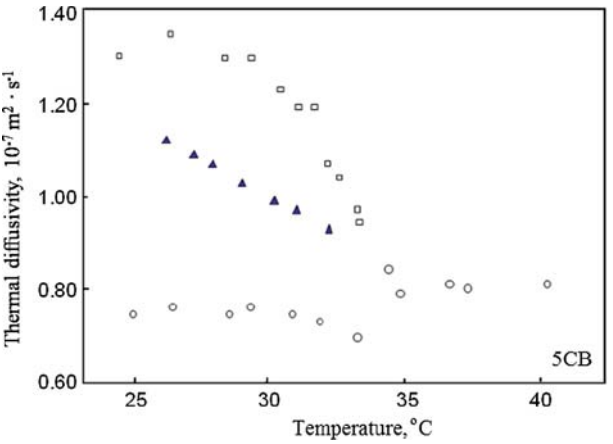

Fig. 3 Thermal-diffusivity coefficient versus temperature for 5CB. *Filled triangles* (randomly) represent data taken from our study, *open squares* (homeotropic) and *circles* (planar) represent data taken from [14]

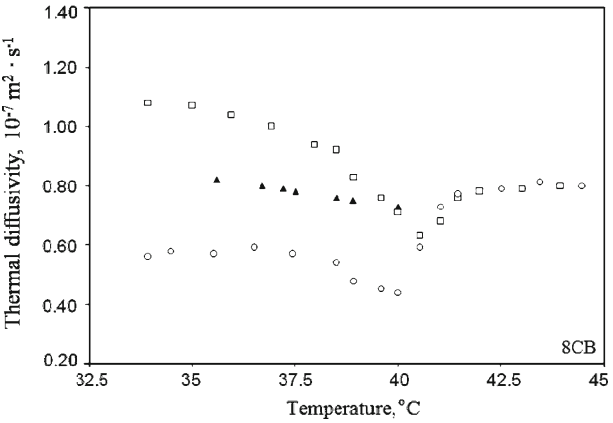

Fig. 4 Thermal-diffusivity coefficient versus temperature for 8CB. *Filled triangles* (randomly) represent data taken from our study, *open squares* (homeotropic) and *circles* (planar) represent data taken from [21]

temperature range from 35 °C to 40 °C and varied between 0.77×10^{-7} m$^2 \cdot$ s^{-1} and 0.86×10^{-7} m$^2 \cdot$ s^{-1} as seen in Fig. 4.

The values of the thermal-diffusivity coefficients obtained in this study were consistent with literature values that were obtained when the molecular orientation was planar (parallel) and homeotropic (vertical). The thermal diffusivity varied from 0.65×10^{-7} m$^2 \cdot$ s^{-1} to 0.45×10^{-7} m$^2 \cdot$ s^{-1} for planar orientation of the molecules and varied from 1.26×10^{-7} m$^2 \cdot$ s^{-1} to 0.65×10^{-7} m$^2 \cdot$ s^{-1} for homeotropic orientation of the molecules [14,15] for the 5CB sample for the determined temperature range. The thermal diffusivity for the 8CB sample in the literature varied from 0.57×10^{-7} m$^2 \cdot$ s^{-1} to 0.39×10^{-7} m$^2 \cdot$ s^{-1} for planar orientation of the molecules and varied from 1.10×10^{-7} m$^2 \cdot$ s^{-1} to 0.72×10^{-7} m$^2 \cdot$ s^{-1} for homeotropic orientation of the molecules for the investigated temperature range.

Molecular anisotropy, which is determined from molecular order, is a most important characteristic of liquid crystals. The molecular orientation of molecules affects the optical, electronic, and thermal properties of the liquid crystal materials. In thermal applications the anisotropy of molecules also affects primarily the thermal diffusivity and secondarily the thermal conductivity of the liquid crystal materials.

The results from this study which were obtained for randomly oriented molecules show also consistency with other results in the literature [14–21]. This study can be analyzed in detail and can be improved for molecular orientation of nematic liquid crystals at certain directions.

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