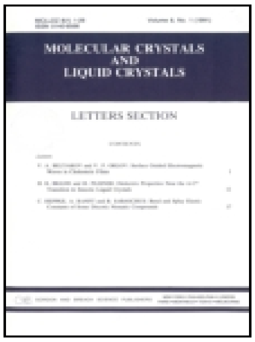

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Determination of Chaotic Behavior in Liquid Crystal

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In this work, chaotic behavior of 4′-(3,7-dimethyloctyloxy)-4-biphenylcarboxylic acid liquid crystal (LC) has been investigated by Schwarzian derivative method. Determination of negative Schwarzian derivative constitutes a sufficient condition for specifying chaotic behaviors mathematically in nonlinear systems. For this purpose, temperature variation of heat flow experimental data of LC has been utilized. In this context, the chaotic behavior of the LC compound has been investigated by means of the Schwarzian derivative. The chaotic behavior on the transition has been mathematically proved for both heating and cooling procedure.

Keywords Chaotic behavior; liquid crystal (LC); phase transition; Schwarzian derivative

1. Introduction

Liquid crystal (LC) science has grown tremendously in recent years for fundamental scientific reasons and widespread LC applications in industry and technology, e.g., display devices, optical devices, and biological sensors. LCs can be grouped into several types, which lead to a variety of phases. The nematic phase is the least-ordered liquid crystalline phase, being characterized by only long-range orientational order. Most of the other liquid crystal phases are smectics which are characterized by varying degrees of positional order and the molecules organize themselves in layers. There are many types of smectic phases, indicated as SmA, SmB, SmC, etc., which differ in the orientation of the preferred direction of the molecules with respect to the layer normal and the distribution of the centers of the molecules within the layer.

The LCs derived from the rod-shaped molecules are called "calamitics." The rod-like molecules are well investigated and extremely useful for the practical applications. This class of materials has various structural and physical properties. Parameters have an effect on the mesomorphic and physical properties of liquid crystals [1–5]. Therefore, the investigation of the connection between type of molecules and the mesomorphic and physical properties of materials is significantly important for the selection of the suitable material

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[6–9]. On the other hand, liquid crystals are the objects of intensive investigations during the last few decades. Therefore, LCs are sufficiently interesting materials for scientific investigations and very perspective materials for technological applications [10,11]. In addition to numerous technological applications, the mathematical theory of liquid crystals is still very rich in the context of phase transitions. For this reason, we have focused on liquid crystal phase transitions.

The phase transition is defined as the transformation of a system from one phase to another. During a phase transition, certain properties of the system change as a result of alteration of some external condition such as temperature, pressure, etc. For the first time, the liquid crystal phase transitions have been discussed in chaotic perspective based on Schwarzian derivative method [12–14], which is utilized for detection of chaotic transitions mathematically. Since LC compounds exhibit properties of liquids and solid crystals, they set a suitable frame of reference for searching chaotic transitions.

Since both mechanical and optical properties of liquid crystals are highly nonlinear [15], the association between the concepts of chaos and liquid crystals produces an interesting phenomenon for almost 20 years. There have been some works focused on the investigation of chaos in liquid crystals by applying electric and magnetic fields [15–17]. There is no scientific investigation for liquid crystal phase transitions as chaotic behavior. In this respect, liquid crystal phase transitions have been analyzed in the context of chaotic behavior based on Schwarzian derivative method.

2. Experimental and Theoretical Details

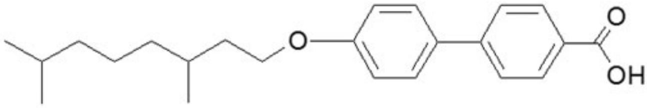
2.1 Synthesis of Liquid Crystal (LC)

The compound (4′-(3,7-dimethyloctyloxy)-4-biphenylcarboxylic acid) (LC) was synthesized by our group [18] with using known procedures [19]. First, ethyl 4′-(3,7-dimethyloctyloxy)-4-biphenylcarboxylate was obtained by the reaction of ethyl 4′-hydroxy-4-biphenylcarboxylate with the 3,7-dimethyloctyl-1-bromide, which was prepared from 3,7-dimethyl-1-octanol (Aldrich, 99.0%), as described previously, using K_2CO_3 as base and 2-butanone as solvent. Then, the hydrolysis reaction of the ethyl 4′-(3,7dimethyloctyloxy)-4-biphenylcarboxylate in EtOH with KOH as base yielded the LC compound. The crude product was purified by crystallization from EtOH. The structure of LC was characterized using various spectroscopic methods (^{1}H-, ^{13}C-NMR, and mass). The proposed structures are in full agreement with these spectroscopic data. Spectroscopic data and mesomorphic data for the LC were given by Ocak et al. [18].

2.2. Mesomorphic Properties of Liquid Crystal

The investigations by polarizing microscopy showed that the LC exhibits liquid crystalline properties as it exhibits a thermotropic enantiotropic mesophase between 163 °C and 225 °C. The phase transition temperatures and enthalpies of the LC are shown in Fig. 1. These mesophases are displayed by typical textures in Fig. 2. As seen from this figure, LC shows SmI and N mesophases in a very small temperature interval.

The Differential Scanning Calorimetry (DSC) data of the LC confirm the phase transition temperatures (see Fig. 3).



T/°C [ΔH kJ/mol]
Cr 163 [*14.1*] Sm I 223 N 224 [*12.2*] Iso

Figure 1. The chemical structure and phase transition temperatures T (°C) of LC (Perkin-Elmer DSC-7; heating rates 10 K min^{-1}; enthalpy value ΔH given behind the phase transition temperatures in italics in square parentheses (kJ mol^{-1}); abbreviations: Cr = crystalline, SmI = smectic I phase, N = nematic phase, Iso = isotropic liquid phase).

2.3. The Schwarzian Derivative for Determining the Chaotic Behaviors in Liquid Crystal Phase Transitions

The investigation of chaotic behaviors of phase transitions of LC systems is based on the fundamental realties of nonlinear dynamic systems given below.

Nonlinear dynamic systems show complex behavior that is often repeated but never in exactly the same way. In this respect, liquid crystal phase transitions can be considered as chaotic behavior phenomenologically, since the temperatures at which phase transitions occur do not coincide with heating and cooling process. Moreover, one of the most crucial intrinsic properties of chaotic systems is that the state of the system can be affected by small variations of its parameters. From this point of view, small changes in temperature parameter for the liquid crystal system manifest itself as an occurrence of the transition from liquid crystal to isotropic phase and vice versa. So that due to reasons mentioned above, phase transitions in LC systems can be examined in the context of chaotic approach.

From this point of view, small variations of temperature, which drives the transition between crystal–liquid crystal and liquid crystal–isotropic phases, can be investigated by means of derivative process, since the derivative of a function represents an infinitesimal change in the function with respect to temperature. So the derivative process is the most appropriate mathematical tool to detect chaotic behaviors. In this context, the Schwarzian derivative method has been utilized to find a sufficient condition for the chaotic behaviors

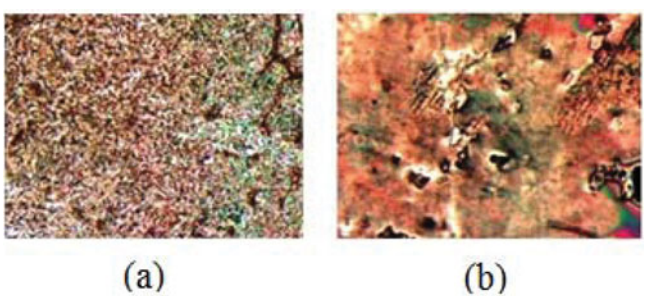


Figure 2. Optical photomicrographs of mesophases of LC as observed on cooling between crossed polarizers. (a) SmI mesophase at 198.8°C; (b) N mesophase at 224.0°C.

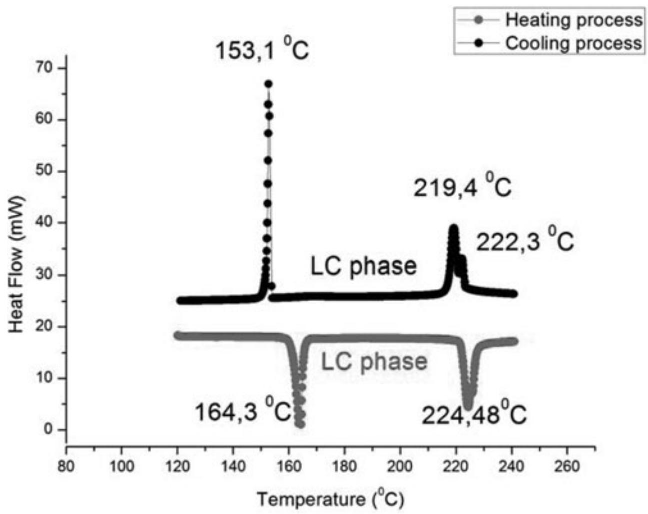


Figure 3. DSC thermogram during the second heating and cooling process for LC (10 K min^{-1}).

[13]. Such chaotic behavior has also been determined by Schwarzian derivation method for superconducting transition [14].

The Schwarzian derivative of a locally univalent analytic function f at point x, $Sf(x)$, is defined by

$$Sf(x) = \left(\frac{f''(x)}{f'(x)}\right)' - \frac{1}{2}\left(\frac{f''(x)}{f'(x)}\right)^2, \tag{1}$$

where $f(x)$is a function with one variable, $f'(x)$ and $f''(x)$ are its first and second continuous derivatives, respectively. The Schwarzian derivative is named for the German mathematician Hermann Schwarz for studying complex valued functions, but it was used for hyper geometric differential equations by Kummer and Reine in 1836 [20, 21].

In 1980s, the Schwarzian derivative was used to limiting the behavior of dynamical systems [22, 23]. According to Katz and Hacıbekiroğlu et al., when the system behaves chaotically, the Schwarzian derivative of the function is negative [12, 13]. Moreover, eventual negative Schwarzian derivative has also been utilized for searching chaotic behaviors in neuroscience especially explaining the electrical activity in neural cells in behavior described as "bursting" [24, 25].

The chaotic behavior in liquid crystal phase transitions has been investigated by heat flow versus temperature data, which has been given in Fig. 3. The Schwarzian derivatives of the heating and cooling process of $HF = f(T)$ have been calculated by Equation (2):

$$S\,[HF(T)] = \frac{HF(T)'''}{HF(T)'} - \frac{3}{2}\left(\frac{HF(T)''}{HF(T)'}\right)^2, \tag{2}$$

where $HF\,(T)'$, $HF\,(T)''$, and $HF\,(T)'''$ represent the first-, second-, and third-order derivatives of the heat flow with respect to temperature.

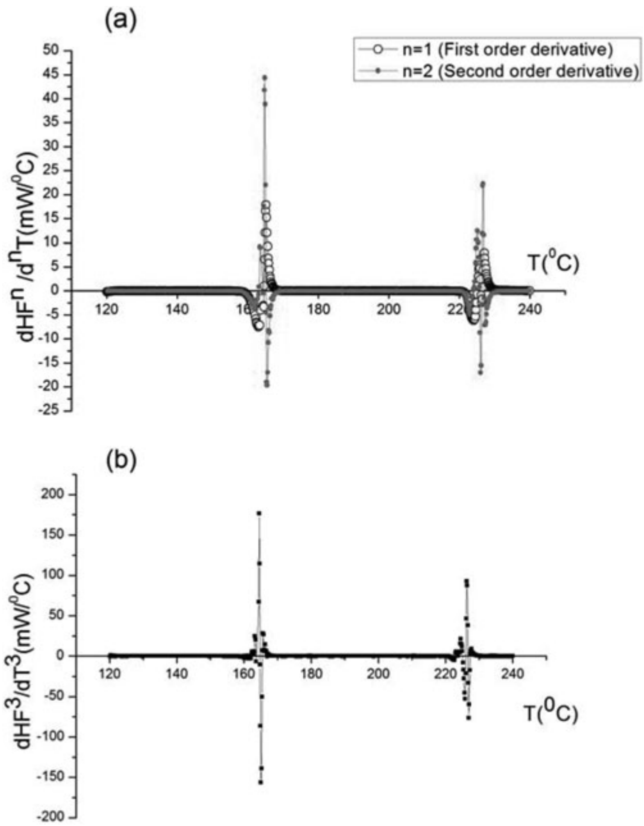


Figure 4. (a) The first-, second-, and (b) third-order derivatives of heat flow versus temperature data of heating process for liquid crystal compound.

3. Results

The first-, second-, and third-order derivatives of $HF\ (T)'$, $HF\ (T)''$, and $HF\ (T)'''$ have been calculated by Origin Lab 8.0 graphic program. The temperature variation of the related

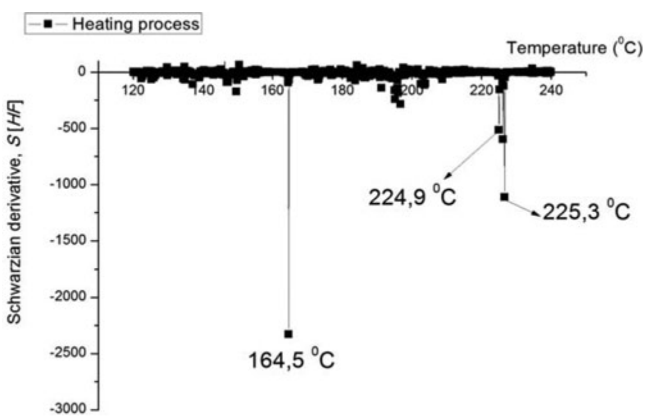


Figure 5. The Schwarzian derivative versus temperature curve of heating process of DSC data.

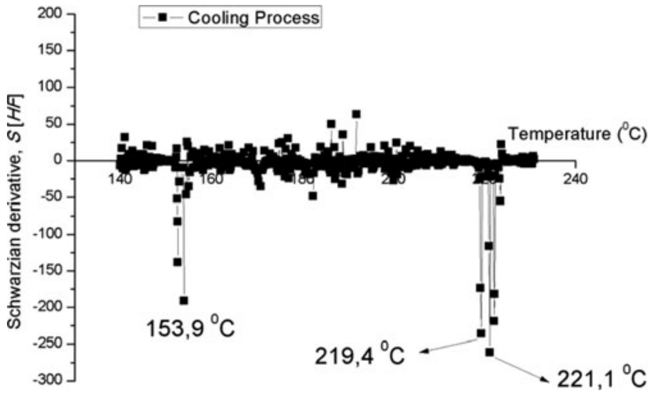


Figure 6. The Schwarzian derivative versus temperature curve of cooling process of DSC data.

derivatives of heating process has been given in Figs. 4(a) and (b). The same calculation procedure has been carried out for cooling process, as well.

According to Equation (2), the Schwarzian derivatives of heating and cooling process have been calculated and given in Figs. 5 and 6, respectively.

As is seen in Fig. 5, Schwarzian derivative has sharp negative peaks at 164.5°C and 225.3°C temperatures at which crystal–liquid crystal and liquid crystal–isotropic liquid phase transitions occur, respectively. These negative and sharp Schwarzian derivative peaks are attributed to chaotic transitions for heating process. Moreover, the Schwarzian derivative of cooling process also agrees with DSC data of LC compound. The sharp negative Schwarzian derivative peaks have been determined at 153.9°C, 219.4°C, and 221.1°C, which are also agree with phase transition temperatures observed in DSC thermogram data given in Fig. 3.

4. Conclusions

In this work, phase transition occurs in LC system has been proposed as a chaotic behavior for the first time. Moreover, the proposal has been confirmed mathematically by determining sharp negative Schwarzian derivative peaks from the DSC data of the LC compound. This mathematical insight can be used for the optimization of modern liquid crystal devices and the design of new devices for specific applications, necessitating continuous cross-disciplinary collaborations between theoreticians, experimentalists, and industrial researchers.

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