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DETERMINATION OF PHASE TRANSITIONS IN HYDROGEN BONDED COMPLEXES (NOBA: PFOA) USING TEXURAL IMAGE PROCESSING TECHNIQUES

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ABSTRACT

Synthesis and characterization of a novel series of inter molecular hydrogen bonded liquid crystals are done. Eleven hydrogen bonded complexes are characterized by the polarizing microscope (POM) attached with a hot stage, Differential scanning calorimeter (DSC) and Fourier transformed infrared spectroscopy (IR). The effect of chain length on the phase transitions is discussed by POM and DSC respectively. The complexes having chain number n=7-12 exhibits nematic, smectic-B and smectic-G. In this case both smectic-B and smectic-G phases are induced by the quenching of smectic-C phase. Along with DSC results, we have done textural analysis using image processing techniques and found that transition temperatures in both the cases are almost identical. We reported corresponding simulated statistical analysis data in comparison with DSC measurements available.

Keywords: hydrogen bonding, differential scanning calorimeter (DSC), smectic phase, statistical analysis, image processing techniques.

1. INTRODUCTION

Image texture, defined as a function of the spatial variation in pixel intensities (gray Values), is useful in variety of applications and has been a subject of intense study by many researchers. One immediate application of image texture is the recognition of image regions using texture properties [1-2]. Texture is the most important visual cue in identifying different types of homogeneous regions. This is called texture classification. The goal of texture classification then is to produce a classification map of the input image where each uniform textured region is identified with the texture class it belongs. We could also find the texture boundaries even if we could not classify the textured surfaces. This is then the second type of problem that texture analysis research attempts to solve texture segmentation [3-5]. In this paper, texture analysis is doing by finding statistical parameters like mean, standard deviation, entropy and energy for nOBA: PFOA compounds. Graphical representation of these parameters in comparison with standard DSC results is proposed and presented.

The hydrogen bonding will place an important role to enhance the liquid crystal character. Most of the researchers done their research work on hydrogen bonding liquid crystals because mesogenic behavior of the compounds [6-13]. The hydrogen bonded liquid crystals first introduced by Kato *et al* [14, 15]. The hydrogen bonded liquid crystals involving inter molecular hydrogen bonding between mesogenic *p-n*-alkoxy benzoic acids (nOBA) with varying chain number from n = 4 to 12 and 16 and non mesogenic perfluoro octanoic acid(PFOA) are synthesized [16]. In this series the lower homologues (n=3-6) and compound having chain number n=16 are found to exhibit monovariant nematic phase whereas the remaining compounds of the series are found to exhibit trivariant liquid crystalline phases with manifestation of smectic B and G phases along with nematic with the quenching of smectic-C phase. The molecular structure of the compound is given below.



PFOA AND ALKOXY BENZOIC ACID



2. EXPERIMENTAL

The compounds *p*-*n*-alkoxy benzoic acids and per fluoro octanoic acid were supplied by Sigma aldrich (Labour Chemikalein GmbH, Seelze, Germany) and the solvents used in the present work are of Merck AR grade. The solid state (KBR) IR spectra were recorded on a Perkin-Elmer FT-IR spectrometer (Perkin Elmer FTIR Spectrum Two, Waltham, MA, USA). The optical textural observations were carried out by S. D. Techs (Machilipatnam, India) polarizing microscope (POM) equipped with digital camera and hot stage. The color images are collected with good resolution and stored in the PC to simulate them with image processing techniques in MATLAB. The transition temperatures and corresponding

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enthalpy values are recorded on a Perkin Elmer diamond DSC (Differential Scanning Calorimeter).

3. RESULTS AND DISCUSSIONS

3.1 Local Binary Pattern

Local Binary Patterns (LBP) are introduced as a powerful local descriptor for microstructures of images. LBP is a simple yet efficient operator to describe local image pattern, and it has achieved impressive classification results on representative texture databases [17]. LBP has been adapted to many other applications, such as face recognition, dynamic texture recognition and shape localization. However, the LBP has a limitation that LBP histogram is calculated over the whole texture image represents only the occurrences of the patterns without any indication about their position. To overcome this problem, we propose a novel representation, called co-occurrence matrix of local average binary pattern (CoLABP), and the authors applied it to texture classification. Co-occurrence matrix of LABP image extracts the features based on local neighborhood of image which contains all spatial and texture feature information of different patterns [18-24]. Parameters extraction from the CoLABP of texture is a helpful process to identify the textural features and it changes either with or without temperature, efficiently in order to investigate the phase transitions of the samples specially the liquid crystals.

In this paper, we propose a multispectral method named as colour co-occurrence local average binary pattern (CCoLABP) by considering the correlations between the colour bands while computing the colour texture features. Here, comes the liquid crystal textures and their change with temperature and provide an opportunity to test the phase transitions and the temperatures at which these transformations occur.

3.2 Software simulation technique

The statistical parameters like mean, standard deviation, energy and entropy is calculated from the standard formulas and results obtained on nOBA: PFOA is presented from Figure-1 to Figure-20.

Mean: The first color moment can be interpreted as the average color in the image, and it can be calculated by using the following formula,

$$E_i = \frac{1}{N} \sum_{j=1}^{N} p_{ij} \tag{1}$$

Where N is the number of pixels in the image and p_{ij} is the value of the *j*th pixel of the image at the *i*th color channel.

Standard Deviation: The second color moment is the standard deviation, which is obtained by taking the square root of the variance of the color distribution.

$$\sigma_{i} = \sqrt{\frac{1}{N} \sum_{j=1}^{N} (p_{ij} - E_{i})^{2}}$$
(2)

Energy:
$$E = \sum_{i=1}^{n} \sum_{j=1}^{m} [CoLABP(i, j)]^2$$
 (3)

Entropy:

$$H = \sum_{i=1}^{n} \sum_{j=1}^{m} \text{CoLABP}(i, j) \log [\text{CoLABP}(i, j)]$$
(4)



Figure-1. Statistical parameters of 4Oba: PFOA Cooling, using Image Processing Technique in Matlab.



Figure-2. Statistical parameters of 40ba: PFOA Heating, using Image Processing Technique in Matlab.

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Figure-3. Statistical parameters of 50ba: PFOA Cooling, using Image Processing Technique in Matlab.



Figure-4. Statistical parameters of 50ba: PFOA Heating, using Image Processing Technique in Matlab.



Figure-5. Statistical parameters of 6Oba: PFOA Cooling, using Image Processing Technique in Matlab.



Figure-6. Statistical parameters of 60ba: PFOA Heating, using Image Processing Technique in Matlab.



Figure-7. Statistical parameters of 70ba: PFOA Cooling, using Image Processing Technique in Matlab.



Figure-8. Statistical parameters of 70ba: PFOA Heating, using Image Processing Technique in Matlab.



Figure-9. Statistical parameters of 80ba: PFOA Cooling, using Image Processing Technique in Matlab.

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Figure-10. Statistical parameters of 80ba: PFOA Heating, using Image Processing Technique in Matlab.



Figure-11. Statistical parameters of 9Oba: PFOA Cooling, using Image Processing Technique in Matlab.



Figure-12. Statistical parameters of 9Oba: PFOA Heating, using Image Processing Technique in Matlab.



Figure-13. Statistical parameters of 10Oba: PFOA Cooling, using Image Processing Technique in Matlab.



Figure-14. Statistical parameters of 10Oba: PFOA Heating, using Image Processing Technique in Matlab.



Figure-15. Statistical parameters of 11Oba: PFOA Cooling, using Image Processing Technique in Matlab.



Figure-16. Statistical parameters of 11Oba: PFOA Heating, using Image Processing Technique in Matlab.



Figure-17. Statistical parameters of 12Oba: PFOA Cooling, using Image Processing Technique in Matlab.

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Figure-18. Statistical parameters of 12Oba: PFOA Heating, using Image Processing Technique in Matlab.



Figure-19. Statistical parameters of 16Oba: PFOA Cooling, using Image Processing Technique in Matlab.



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Figure-20. Statistical parameters of 16Oba: PFOA Heating, using Image Processing Technique in Matlab.

The present analysis deals with the transition temperatures of Hydrogen boded liquid crystal complexes. Textures of the given compounds are recorded using a polarizing optical microscope. The textures are captured as a function of temperatures, until the sample temperature reaches the isotropic state. On heating noBA: PFOA undergoes a phase transition from the crystalline state to the isotropic state via an intermediate nematic phase. The captured images or textures are stored in database and applied image processing techniques on it to find the statistical parameters. The statistical parameters are computed using equations from (1)-(4) with the help of Matlab software. Once the parameters are computed the plots are drawn for parameters as a function of temperature (Figures 1 to 20). The abrupt changes in the statistical parameter indicate the consequent changes in the features of the textures of samples with respect to temperature due to the phase transition of the material. Comparative results for both DSC and simulation is presented in Table-1 and observed that approximately equal results in transition temperatures are obtained.

S. No.	Compound	DSC Results		Matlab simulation results	
		Heating	Cooling	Heating	Cooling
1	40BAPFOA	151.66	151.75	151	150.2
2	50BAPFOA	147.60	141.77	148.1	139
3	60BAPFOA	145.06	142.04	145	142
4	70BAPFOA	146.52	96.0, 88.58, 83.0	145.3	94.3, 88.4, 86.2
5	80BAPFOA	136.0	142.0, 99.02, 90.08	137.2	141.2, 99.4, 86.2
6	90BAPFOA	114.57	112.06, 89.88,74.59	114.5	113.7, 88.7, 71.3
7	100BAPFOA	96.76	139.6,117.89, 92.38	98.6	137.1, 119.8, 92.7
8	110BAPFOA	138.51	133.09,124.55,83.26	138.5	132.7, 123.1, 84.2
9	12OBAPFOA	124.63	122.0, 77.33, 67.93	124.6	122.4, 76.7, 68.8
10	16OBAPFOA	121.07	121.0	123.45	121.0

Table-1. Comparison between DSC and Simulated Results of Transition Temperatures.

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Figure-21. Colour LBP image in compound 7oba: PFOA Cooling in Smectic-G phase.



Figure-22. Colour LBP image in compound 9oba: PFOA Cooling in Nematic phase.



Figure-23. Colour LBP image in compound 8oba: PFOA Cooling in Smectic-B phase.

CONCLUSIONS

The experiment is carried out on both cooling and heating cycles and the plots are drawn for all the cases. The observed results from simulation are in very good agreement with standard DSC results. From the obtained results we can conclude that, this is one of the accurate measurement techniques for finding the phase transitions of the liquid crystalline compounds, along with other techniques that are available.

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