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Features of the transition to the isotropic state of the liquid crystal sensitive element of the gas sensor under the action of acetone vapor

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The process of detailed research of the transient process, which takes place in the sensitive element of the liquid crystal sensor during interaction with acetone vapors, is described. The abrupt transition of the liquid crystal to the isotropic state is one of the main obstacles which prevents the construction of an acetone liquid crystal sensor. A mixture of nematic liquid crystal E7 and cholesteric impurity CB15 was used as a sensitive element

Keywords: gas sensor, acetone vapor, sensitive element.

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Introduction

Liquid crystal gas sensors today are promising compact solutions for determining the concentrations of marker substances in gas mixtures [1]. Today, the main method of determining the concentrations of such substances in gas mixtures is mass spectrometry, which requires the presence of qualified personnel for measurements, and is also time-consuming. One of the main applications for such sensors is medicine, so the marker substances should be associated with a change in the state of the human body [2-5].

In general, a suitable marker of the disease can be almost any substance that appears outside the normal state in the exhalation gases, is related to the process of a particular disease or pathology, and is available for detection by modern technical means [6-8].

Acetone is one of the most noticeable and easy to identify markers, which may indicate a violation of the body, in particular diabetes mellitus [9-11]. In the presence of diabetes mellitus in the body as a result of fatty acid oxidation, an excess of acetone is produced [12, 13]. In a healthy state, the concentration of acetone in exhalation is from 0.39 to 0.85 ppm, and in diabetes can be from 2.2 to even 400 ppm. An increase of its concentration can be detected both in the patient's blood and in the exhaled air [14-16]. The studied sensory system can determine its concentration in a mixture of exhaled gases. To date, we have a large number of studies on the interaction of liquid crystal sensitive elements with acetone vapors [17,18].

A series of sensors whose active substance is a liquid crystalline substance was developed in [19-21]. The basis of such sensors is the change in the wavelength of the transmission from the concentration of the analyte and it can be used to identify chemicals vapors. In the review [22] a wide range of optical sensors active environments based on liquid crystalline substances is given. These sensors are highly sensitive but may be cross-sensitive to similar structure molecules. Our proposed sensor based on liquid crystalline substances is highly sensitive, compact and easy to use.

I. Sensitive Element

In previous studies on the interaction of the liquid crystal sensitive element with acetone vapor, it was possible to record the response of the sensor to the presence of a marker substance. However, with increasing concentration of acetone in the gas mixture revealed an abrupt dependence, which indicates a sharp transition of the sensitive element to the isotropic state. A similar sharp transition process was obtained in [18].

The sensitive element of the sensor is a mixture of nematic liquid crystal E7 with optically active cholesterol impurity CB15. The main operating principle of the liquid crystal sensitive element is to change the spectral characteristics of the liquid crystal mixture under the action of acetone vapor [23].

E7 is a four-component liquid crystal mixture based on cyanide liquid crystals [24]. It consists of liquid crystals 5CB, 7CB, 8OCB, 5CT. The composition of the mixture is shown in Fig. 1. The presence in the mixture of four types of molecules with different molecular sizes and properties allows us to distinguish such a mixture as promising for research.

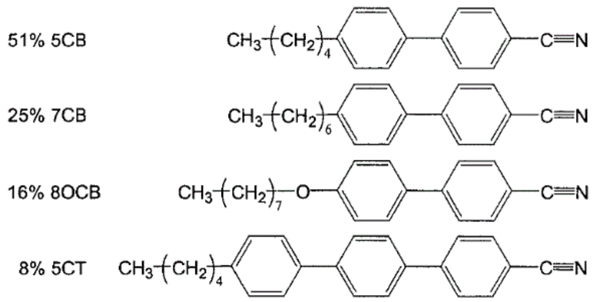

Fig. 1. Percentage composition of the E7 mixture.

CB15 - (4- (2-methylbutyl) -4-cyanobiphenyl) cholesteric liquid crystal used as an optically active impurity.

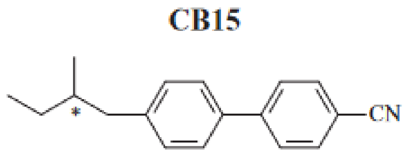

Fig. 2. Structure of cholesteric liquid crystal CB15.

Molecules of the liquid crystal mixture E7 and CB15, as well as acetone can be characterized by a significant dipole moment, which causes a dipole-dipole interaction between molecules and leads to a rapid transition of the liquid crystal mixture to an isotropic state.

Nematic mixture E7 consists of 4 components that have a similar chemical structure (4-alkyl-4'-cyanobiphenyls or terphenyls) so there is no specific interaction between the components. As a result, we consider E7 as a single almost homogeneous nematic matrix.

The chiral impurity CB15 also has a similar molecule structure, so we can assume that CB15, although it induces helical twisting in the system, but does not make any significant changes in the orientational ordering. Therefore, we can consider the system E7 + CB15 as qualitatively homogeneous, in terms of orientation. In fact, we have a cholesterol matrix that will interact with acetone.

Consider the process of interaction of a cholesterol mixture with acetone. Under the action of acetone vapors, the step of the cholesteric spiral changes, which is described by expression (1), which describes the change of the step of the spiral in the first approximation. The impurity is not optically active (acetone vapor) and does not interact chemically with the matrix.

$$p^{-1} = p_0^{-1}(1-w) + k_p w(1-w) + p_d^{-1} w \qquad (1)$$

A detailed description of the effect of absorbed acetone vapor on the pitch of the cholesterol spiral is considered in book [25].

As the concentration of acetone vapor increases and the critical concentration is reached, the orientation parameter decreases so much that there is a transition to the isotropic phase. After some time, the acetone evaporates and the value of w in the above formulas will decrease - up to 0, and there will be a reverse phase transition to an orientationally ordered cholesteric phase. The color of the liquid mixture will be restored.

At the first stage, when little acetone vapor is absorbed, and its amount is insufficient to achieve an isotropic transition by the formula:

$$v = v_0(1-w) + k_v w(1-w) + v_d w \qquad (2)$$

then the pitch of the spiral will change (ie, λ_{max}).

This is described by the formulas:

$$\Delta p^{-1} = \left(\gamma T \frac{\partial p_0^{-1}}{\partial T} - p_0^{-1} + k_p\right) w - \left(\gamma T \frac{\partial p_0^{-1}}{\partial T} + 2k_p\right) \frac{w^2}{2} \qquad (3)$$

$$\Delta p = \gamma T \frac{\partial p}{\partial T} w \qquad (4)$$

If we do not achieve an isotropic transition, then gradually, after isolating the system from the effects of acetone vapor, the initial values of p (λ_{max}, color) should be restored.

This process is the basis of the liquid crystal sensor.

II. Hardware Part of the Sensor

The measurements were performed using a hardware-software complex, which provides intensities measurement of the three spectral components of light that passing through the liquid crystal sensitive element.

Fig. 3 shows 1 - optical emitters; 2 - receiving module with photodiodes (TCS34903); 3 - tank for marker substances; 4 - sensitive liquid crystal element; 5 - system on chip; 6 – the personal computer.

The general principle of operation is the transmission of light from the radiating element through the liquid crystal sensitive element, which under the action of the marker substance gradually makes the transition to the isotropic state. The corresponding change in the transmittance of the sensitive element is registered by the receiving module with photodiodes. The photodiode module allows to determine the transmission intensities separately for the three spectral components. Information from the receiving module is sent to the microcontroller, and then through the usb interface to a personal computer, where the data is displayed using special software.

III. Experiment

On the basis of the developed hardware-software complex for the character analysis of transition of liquid crystalline substance under the influence of acetone vapors we investigated character of change of a step of a cholesteric spiral during transition process to an isotropic state.

The obtained graphs clearly reflect the transients stretched over time, in contrast to the results in [4,5]. In Fig. 3, a change in the transmittance intensity for the three spectral components can be observed under the action of a small concentration of acetone vapor. The maximum values of the transmission intensities are reached after 5 minutes of measurement, where the liquid crystalline mixture is completely converted into an isotropic state.

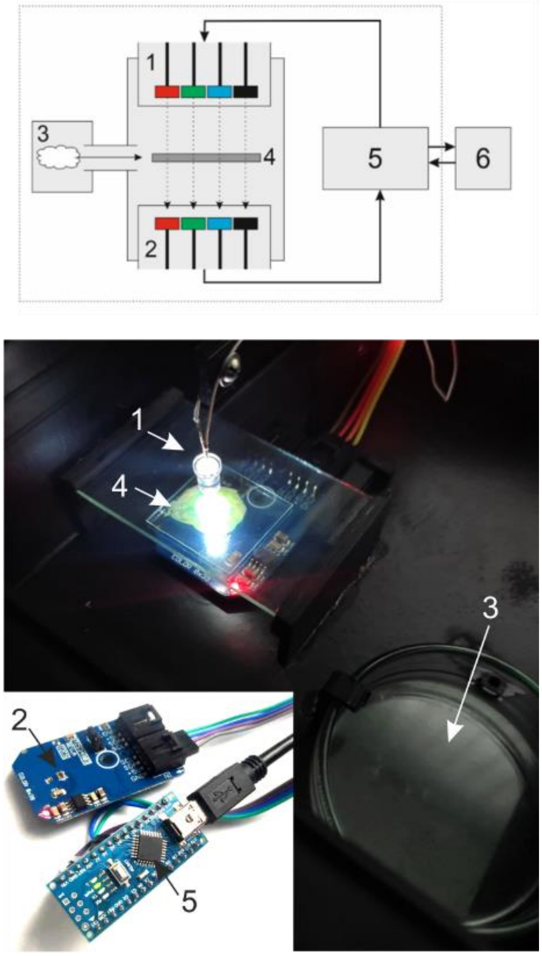

Fig. 3 The structure of the hardware and software complex for the study of the characteristics of liquid crystal sensitive elements

Curves of changes of spectral characteristics in fig. Fig. 4 shows the measurement of the change in the transmittance of the liquid crystal element at a concentration of acetone vapor of about 120 ppm. In comparison with the previous measurement, it is worth noting the similar behavior of the change in the intensity of all spectral components, as well as the reduction of the time required to achieve the isotropic state. In this experiment, peak transmission values are reached in 3 minutes of measurements.

The latest measurements of the interaction of the liquid crystal sensitive element and acetone vapor were performed at an acetone concentration of about 240 ppm and are shown in Fig. 5. Here, as in the previous case, it is necessary to pay attention to the characteristic appearance of the measured curves of the intensity change, as well as, accordingly, the change in the time of reaching the isotropic state by the liquid crystal. In particular, in this measurement, saturation and the transition to the isotropic state occurs 2 minutes after the introduction of acetone.

According to visual observations of changes in the state of the liquid crystal during the experiment, we can talk about the complete transparency of the liquid crystal mixture in each measurement, which indicates the transition to the isotropic state. The main difference for different concentrations of acetone is the time required to achieve an isotropic state by the liquid crystal mixture.

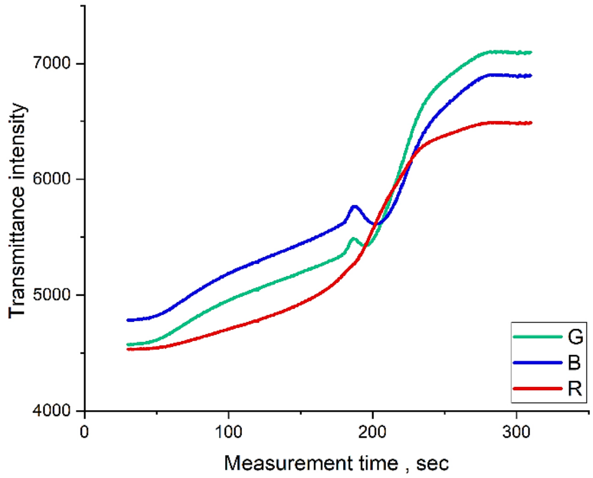

Fig. 4. Acetone concentration 0.1ml (60 ppm).

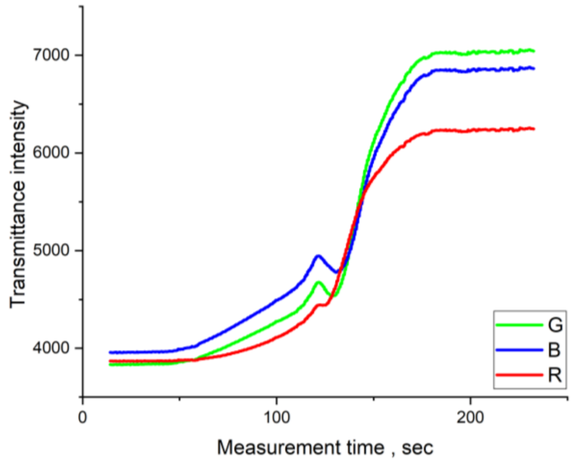

Fig. 5. Concentration of acetone 0.2 ml (120 ppm).

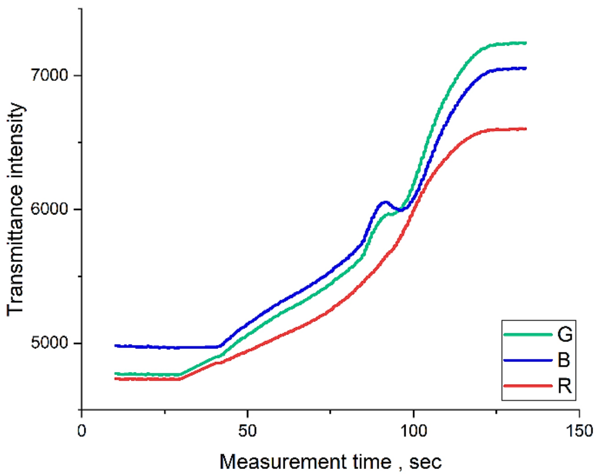

Fig. 6. Concentration of acetone 0.4 ml (240 ppm).

Based on the measurements, a graph of the dependence of the time of transition of the liquid crystalline mixture to the isotropic state on the concentration of acetone was constructed (Fig. 7). Accordingly, with increasing concentration of acetone, the time required for the transition to the isotropic state decreases.

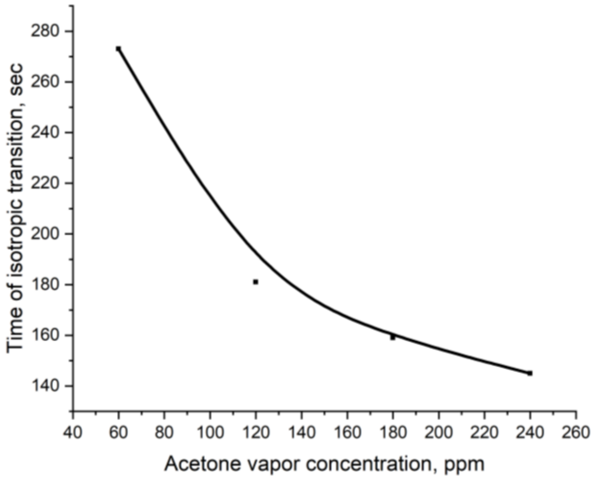

Fig. 7. The dependence of the transition time to the isotropic state on the concentration of acetone

The applied new cholesteric-nematic liquid crystalline mixture shows good results as a sensitive element for determining the concentration of acetone vapor.

Conclusions

The investigated liquid crystal sensitive element shows a clear dependence of the isotropic state transition rate depending on the concentration of acetone. In contrast to previous studies, we were able to achieve a gradual rather than abrupt transition of the liquid crystal mixture to an isotropic state under the action of acetone vapor, which is a good basis for further development of the sensor. In addition, this study demonstrates changes in individual spectral components, which allows us to more fundamentally determine the changes in bandwidth depending on the analyte.

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Особливості методики дослідження перехідного процесу рідкокристалічного чутливого елементу газового сенсора в ізотропний стан під дією парів ацетону

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Описано процес детального дослідження перехідного процесу, який відбувається в чутливому елементі рідкокристалічного сенсору при взаємодії з парами ацетону. Стрибкоподібний перехід рідкого кристала в ізотропний стан є однією з основних завад, що заважає побудові рідкокристалічного сенсора ацетону. В дослідженні в якості чутливого елементу використано суміш нематичного рідкого кристалу Е7 та холестеричної домішки СВ15.

Ключові слова: газовий сенсор, пари ацетону, чутливий елемент.