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Identification of Chemical Compounds Spectra with the Help of Coherent Optics Methods

A short description of coherent optical system designated for the identification of chemical compound spectrum is given. The value of the respective correlation function is assumed to be a measure of the similarity among the spectra.

1. Introduction

The present paper deals with a method of holographic filtration used for determining the degree of similarity among the spectra of several chemical compounds and for ordering them according to the similarity degree of particular details. The procedure proposed is based largely on the work [1], performed at the Institute of Automatics of the Academy of Sciences, Novosybirsk, USSR. As the method proved to offer wide applications in many fields (e.g. recognition of metallographic structures recorded on microphotographs, identification of persons exhibiting certain external features, finger prints identification etc., it seems that the modified version of the method, presented below, may be useful in solution of many problems.

2. Theoretical Basis of the Method

We take use of the correlation method of subject recognition given in [2, 3]. This method allows to performe the following operations:

a) Matched Filter Recording [4]

$$G = |\mathfrak{F}\{h(x,y)\}+\exp(i\omega_x a)|^2 = |H(\omega_x,\omega_y)|^2+1+H(\omega_x,\omega_y)\exp(-i\omega_x a)+ +H^*(\omega_x,\omega_y)\exp(i\omega_x a),$$

where $\mathfrak{F}\{\}$ — a symbol of Fourier-transforming operation,

$h(x,y)$ — object function for which the matched filters is to be produced,

ω_x,ω_y — components of the spatial frequency ω in the x and y directions,

a — inclination factor of the reference beam with respect to the optical axis of the system performing the Fourier transform operation on the object function $h(x,y)$

$$H(\omega_x,\omega_y) = \mathfrak{F}\{h(x,y)\},$$

$H^*(\omega_x,\omega_y) = \mathfrak{F}^*\{h(x,y)\}$ — the required matched filter.

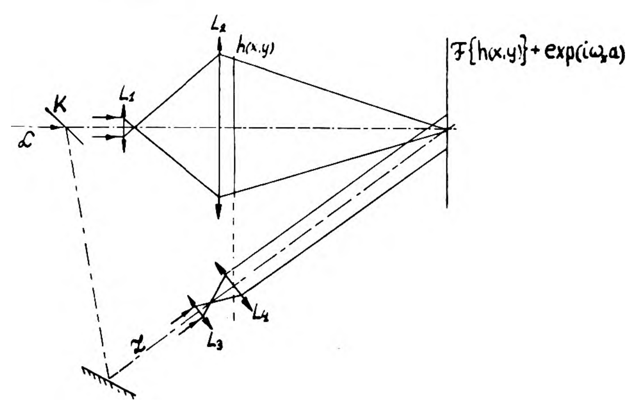

Fig. 1. Scheme of the setup for matched filtres production a—He-Ne laser beam, K — beam splitter, L_1 — condenser, L_2 — optical object analyser, L_3 and L_4 — the optical systems forming the reference beam h (x, y) — pattern functions

An experimental realization of the holographic recording of the matched filters is shown in Fig. 1.

b) Recognition in the Optical Correlator

The Fourier-transformation of the examined object function $f(x,y)$ and multiplication of its spatial spectrum by the frequency response of the matched filter yield

$$\mathfrak{F}\{f(x,y)\}H^*(\omega_x,\omega_y) = F(\omega_x,\omega_y)\cdot H^*(\omega_x,\omega_y).$$

An inverse Fourier transformation gives

$$\mathfrak{F}^{-1}\{F(\omega_x,\omega_y)\cdot H^*(\omega_x,\omega_y)\} = f(x,y)\star h(x,y),$$

where

$f(x,y)$ — comparative information contained in the matched filter of the pattern function $h(x,y)$,

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$\mathfrak{F}\{f(x,y)\} = F(\omega_x,\omega_y)$,

$\mathfrak{F}^{-1}$ — symbol of inverse Fourier transformation,

$*$ — symbol of correlation operation.

In the case of square-law detector (e.g. photographic detection, photoelectric detection) the effect is proportional to

$$\left| f(x,y) * h(x,y) \right|^2_{\substack{x=0 \\ y=0}}.$$

In general this expression takes the maximum value for

$$f(x,y) = c \cdot h(x,y),$$

where c is a constant.

An experimental realization of the recognition process is illustrated in Fig. 2.

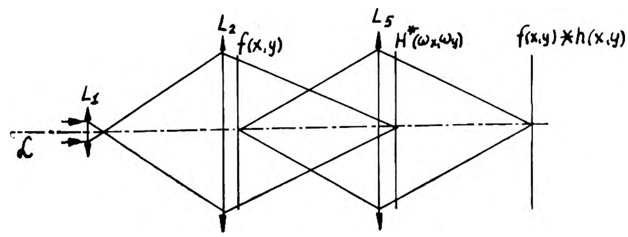

Fig. 2. Scheme of the optical system of the correlator. a — He—Ne laser beam, L_1 — condenser L_2 — optical object analyser, $f(x,g)$ — object under test, L_5 — reconstructing lens, $H^*(\omega_x,\omega_y)$ — matched filter, $f(x,y) * h(x,y)$ — correlation operation

In the present paper an integrated holographic filter has been applied. It consists of differential matched filters for a simultaneous or direct registration and of a lens operator. The production method of differential matched filters is given in [5], while the holographic recording of the lens operator is described in the paper [6].

3. Experimental Results

A set of object functions — absorption spectrum curves of several chemical compounds — are made in the form of photographic negatives on the ORWO NP-15 material. The matched filters were recorded on the SCIENTIA 8E75 photographic plates produced by Agfa-Gevaert. The determined values of the auto- and cross-correlation functions are presented in Table.

Determined values of auto- and cross-correlation functions

	Number of object function						
	1	2	3	4	5	6	7
1	1	0.38	0.21	0.33	0.30	0.13	0.19
2		1	0.75	0.35	0.30	0.21	0.37
3			1	0.31	0.44	0.51	0.38
4				1	0.30	0.26	0.30
5					1	0.23	0.38
6						1	0.30
7							1

Relatively high values have been obtained for autocorrelation function. The value of cross-correlation function closest to unity was obtained for the 2 and 3 absorption spectra, which are slightly differing alterations of methyl—2-benzyl—4-isopropyl—5-hydroxybenzen.

4. Conclusion

As mentioned earlier, the experiment was performed in a setup differing somewhat from the schemes described in the literature. The novelty consists in a holographic recording of the lens performing the inverse Fourier transformation and applying the rotating, matched filters, which allow to avoid of the laborous fitting of the orientation of the object and filters, necessary in typical arrangements.

Identification des spectres des composés chimiques au moyen des méthodes de l'optiqe de la lumière coherénte

On a décrit le système optique cohérent servant à indentifier les spectres des composés chimiques. La similitude de ces spectres s'exprime par la valuer des fonctions de corrélation. Le corrélateur optique contient, entre autres éléments, des corrélomètre filtres adaptés et effectués à l'aide de la méthode holographique.

Опознавание спектров химических соединений при помощи методов оптики связного света

Описана когерентная оптическая система для опознавания спектров химических соединений. Мерой подобия этих спектров является значение функции корреляции. В оптическом корелометре имеются, между другими элементами, припасованные фильтры, изготовленные голографическим методом.

References

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