SPECTROELLIPSOMETRIC TECHNOLOGY FOR ECOLOGICAL MONITORING OF THE WATER SYSTEMS

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ABSTRACT

Spectroellipsometry is a peak of polarization optics. The creation of multichannel polarization optical instrumentation and use of spectroellipsometric technology are very important for the real-time ecological control of aquatic environment. Spectroellipsometric devices give us high precision of measurements. Spectroellipsometric multichannel measurements in an aquatic environment provide an information basis for the application of modern algorithms for the recognition and identification of pollutants. New original elements (coaxial polarization switchers and achromatic compensators), developed in IRE RAS, allow to design cheap polarization systems (for example, spectroscopic ellipsometers, polarization spectrometers, polarimeters, dichrometers, polarization microscopes and interferometers, sensitive photometers, differential reflectometers) without expensive standard polarization elements.

1. INTRODUCTION

The creation of multichannel polarization optical instrumentation and use of spectroellipsometric technology are very important for the real-time ecological control of aquatic environment. It should be mentioned that efficient solution of this multiparametric problem greatly depends on the precision and simplicity of ellipsometric devices.

This report is aimed to describe

- A technology of combined use of spectroellipsometry and algorithms of identification and recognition that allowed the creation of a standard integral complex of instrumental, algorithmic, modular and software tools for the collection and processing of data on the aquatic environment quality with forecasting and decision - making functions
- A compact measuring - information multichannel spectroellipsometric system (device) for monitoring the quality of aquatic environment, that is based on the combined use of spectroellipsometry and training, classification, and identification algorithms.

This spectroellipsometric system will differ from modern foreign analogues by the use of a new and very promising method of ellipsometric measurements, an original element base of polarization optics and a complex mathematical approach to estimating the quality of a water object subjected to anthropogenic influence.

Unlike foreign analogues, the system has no rotating polarization elements. This allows one to increase the signal-to-noise ratio and the long-term stability of measurements, to simplify and reduce the price of multichannel spectroellipsometers.

The system will be trainable to the recognition of the pollutants of aquatic environment.

2. MEASIRING COMPLEXES

A spectroellipsometer in laboratories of IRE RAS is designed for in-situ real time measurements of spectra of ellipsometric parameters Psi and Delta with consequent change-over to spectra of transmitted and reflected signal from water media in frames of used physical model of water environment(Fig.1).

A compact measuring - information multichannel spectroellipsometric system (device) is applied for monitoring the quality of natural and waste water, that is based on the combined use of spectroellipsometry and training, classification, and identification algorithms

Figure 1: High precision real-time multi-wavelengths spectroscopic ellipsometer with binary polarization modulation (one of modifications) with registration and recognition system at the base of notebook

2.1. Device composition:

- Polarizer block;
- Analyzer block;
- Power supply unit;
- Illuminator;
- Fiber-optic cabel;
- Notebook with interface unit;
- Wide-band filters/

2.2. Features of high precision real time multi-wavelengths spectroscopic ellipsometers created for monitoring the quality of natural and waste waters

- New approach in ellipsometry, based on binary polarization modulation;
- New low cost effective polarization elements;
- No rotating polarization elements;
- Excellent signal-to-noise ratio and the long-term stability of measurements makes possible to simplify and reduce the price of the multichannel spectroellipsometers;
- One of the key element of the systems is a polarization switch which transforms unpolarized light from a source into highly linearly polarized light with alternate (up to KHz or more) and orthogonal polarizations;
- Sets of silicon photodiodes with arbitrary access to them;

• Flexibility, simple design, low cost, high precision, long term stability.

2.3. Specifications of some spectroellipsometers used:

a) Specification of portable 128-channel spectroellipsometer:

• Spectral range 280-600 nm
• Minimal measurement time 0.5 sec
• Precision and stability 0.01 and 0.02 degree in Psi and Delta, respectively, polarization rotation angle – 0,001 degree
• Sources: miniature pulsed xenon lamp PX-2 with high resource and laser diode
• Micro spot focus 300μm with PX-2 and 30μm with laser diode
• Acromatic compensator
• User-friendly software
• A weight of measuring device – about 4 kg.

b) Specification of compact 128-channel spectroellipsometer with halogen lamp.

• Spectral ranges-380-740 nm and 650-930 nm.
• Minimal measurement time- 0.6 sec.
• Precision to 0.003 and 0.01 degree in Psi and Delta, respectively, polarization rotation angle – 0,001 degree.
• Sources: halogen lamp KGM-9-70
• Long-term stability 0,01 degree
• Use of acromatic compensator on the basis of Fresnel rhomb made of fused quartz enhances precision of measurements.
• A weight of measuring device – about 4 kg.
• Polarization block-2 kg. Analyzer block-2 kg

3. ADAPTIVE IDENTIFIER

For the first time the combined use of real - time spectroellipsometry measurements and data processing methods has been realized in an **Adaptive Identifier.**

3.1. Structure of the Adaptive Identifier:

• The algorithmic support of the Adaptive Identifier is based on a complex application of recognition and classification algorithms on the basis of 128 spectra images registered during a fixed period of time.
• A time interval of 1 second is usually established and provides about 30 value of brightness for each of the 128 optical channels.
• The spectra obtained are sources of set of statistical parameters and different characteristics united into vector spaces for their comparison with the standard samples of famous pollutants stored on the computer.
• The technology of this comparison depends on the diversity of identification methods.

3.2. Learning procedure description

The system is trainable to the recognition of the pollutants of aquatic environment.

Learning procedure includes:

• The Adaptive Identifier is designed to learn from the measurements of spectral characteristics and the simultaneous independent measurement of the content of chemical elements in the aquatic environment.
• As a result, a standard data bank is created in the knowledge base, comparison with which provides the solution of the identification problem. The software of the Adaptive Identifier provides different algorithms for the solution of this problem, and cluster analysis is among of them.

4. MEASURING TECHNIGUE FEATURES

There are some specific features of measurements of the quality of natural and waste water using spectroellipsometric technology:
1. Measurements of natural and waste water quality may be performed using
a) **transmission** scheme when quality of sample is measured during inserting the fused quartz cuvette with water analyzed into spectroeelipsometer device.
b). **reflection** scheme when quality of water is measured by inserting of spectroellipsometer sensor into water media examined.
2 Because of high accuracy of measurements with the spectroellipsometers it is not possible to use whole potential of method for remote measurements of natural and waste water quality (Even small waves, ripples, foam can influence on quality of measurements)

5. APPLICATION

The Adaptive Identifier can be used in different fields where the quality of water should be estimated or the presence of a particular set of chemical elements should be revealed. The Adaptive Identifier solves these problems by real-time monitoring of the aquatic environment. In the stationary version it allows the tracking of the dynamics of water quality in a stream, and when placed on a ship, it allows the measurement of water parameters along the route.

The functionality of the Adaptive Identifier can be extended by increasing the volume of standards in the knowledge base. The use of a natural light source allows the examination of soils, the indication of oil products on a water surface, the determination of the degree of the pollution of atmospheric air and the estimation of the conditions of other objects of the environment, whose spectral images may change.

An adaptive spectroellipsometric technology may be applied to following areas:
- Estimation of natural and wastewater quality;
- Analysis of liquids in medicine, biochemistry, food industry.
- Measurement of the mineralization level and chemical pollution of reservoir depending on the pollution type
- Estimation of water salinity variations
- Ellipsometrically based biosensor and gas sensor systems
- Testing the organic pollution clots in water enviroment

6. EXPERIENCE

The Adaptive Identifier was tested under expeditionary conditions on board of the research vessel "Dmitry Mendeleev" in the Japanese Sea and in central areas of the Pacific Ocean and also during the investigation of aqueous systems of South Vietnam and Siberia (lake Baikal, Angara and Yenisey river) within the framework of the Russian - American and Russian - Vietnamese ecological expeditions.

A Russian - Vietnamese scientific and engineering laboratory has been created to create a standards base and to prepare the Adaptive Identifier for full - scale production.

7. PERSPECTIVES AND OBJECTIVES

The main objective of work is to create in future the compact information systems for monitoring the quality of aquatic environment and to investigate their potential efficiency. These systems are based on the combined application of methods of the spectroellipsometry, and algorithms of training, classification, and identification.

The realization of this objective will require the combined use of engineering and the algorithmic tools providing real - time measurements and data processing..

The technology of combined use of spectroellipsometry and the algorithms of detection and classification will allow the creation of an original system of instrumental, algorithmic, modular and software tools for the collection and processing of data on the aquatic environment with forecasting and decision-making functions.

The theoretical part of the work will include the use of methods of polarization optics, mathematical statistics, the theory of pattern recognition and mathematical modelling.

- creation of a new element base for polarization optics with simple and efficient switches of the polarization state (SPS), that successfully substitutes for the conventional expensive polarizer – modulators of polarization state with rotating polarization elements
- optimization of the spectrum of the ellipsometric method concerning the change of the amplitudes and phases of mutually orthogonal components of electromagnetic radiation for measuring the thickness of thin films on a water surface. Determination of sensitivity and precision limits of adaptive spectroellipsometers in different operating regime
- creation of methods for investigating the water surface, determination of statistical characteristics of "spottiness" as informative signs for solving detection, classification, and identification problems
- elaboration and optimization of algorithms for the detection, classification, and identification of the characteristics of the aquatic environment for adaptive spectroellipsometers. Creation of a bank of standards on the basis of the measurement of the pollution level of the aquatic environment for training the adaptive spectroellipsometer.

The experimental part of the work described in report will include desription:

- the laboratory and on-site measurements of absorption, scattering, and reflection of electromagnetic waves from aquatic objects under local and structural adaptation of the model estimation of the efficiency of the technique, algorithms and models for specific aquatic objects

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