

An adaptive spectroellipsometric technology for ecological monitoring of sea water

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Abstract

Spectroellipsometry is the peak of polarization optics. The creation of multichannel polarization optical instrumentation and use of spectroellipsometric technology are very important for the real-time ecological monitoring of the aquatic environment. Spectroellipsometric devices give us high precision of measurements. Spectroellipsometric and their multichannel measurements in an aquatic environment provide the basis for the application of modern algorithms for the recognition and identification of pollutants (Klimov *et al.*, 2002). New original elements (coaxial polarization switchers and achromatic compensators), developed at the Institute of Radio Engineering and Electronics of the Russian Academy of Sciences, allow the design of inexpensive polarization systems, such as spectroscopic ellipsometers, polarization spectrometers, polarimeters, dichrometers, polarization microscopes and interferometers, sensitive photometers, and differential reflectometers without expensive standard polarization elements.

Introduction

The creation of multichannel polarization optical instrumentation and the use of spectroellipsometric technology are very important for the real-time ecological monitoring of aquatic environment. The ability to handle multiparametric problems in monitoring efficiently greatly depends on the precision and simplicity of ellipsometric devices.

This report aims to describe:

- A technology that combines the use of spectroellipsometry and algorithms of identification and recognition which allows the creation of a standard integral complex of instrumental, algorithmic, modular and software tools for the collection and processing of data on aquatic environment quality, and has forecasting and decision-making functions;
- A compact measuring-information multichannel spectroellipsometric system for monitoring the quality of the aquatic environment that is based on the combined use of spectroellipsometry and training, classification, and identification of 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 body 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 trained to recognize pollutants in the aquatic environment.

Methodology

Methodology consists of:

- A 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 that makes it possible to simplify and reduce the price of multichannel spectroellipsometers,
- One of the key elements of the systems being a polarization switch which transforms unpolarized light from a source into highly linear 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.

Specifications

- a) Portable 128-channel spectroellipsometer:
- Spectral range 280–600 nm,
 - Minimal measurement time 0.5 s,
 - Precision and stability to 0.01 and 0.02 degrees in Psi and Delta, respectively, and polarization rotation angle 0.001 degree,
 - Sources: miniature pulsed xenon lamp PX-2 with high resource and laser diode,
 - Micro-spot focus 300 μm with PX-2 and 30 μm with laser diode,
 - Achromatic compensator,
 - User-friendly software,
 - Weight of measuring device about 4 kg.
- b) Compact 128-channel spectroellipsometer with halogen lamp:
- Spectral ranges 380–740 nm and 650–930 nm,
 - Minimal measurement time 0.6 s,
 - Precision to 0.003 and 0.01 degrees 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 an achromatic compensator on the basis of Fresnel rhomb made of fused quartz that enhances the precision of measurements,
 - Weight of measuring device about 4 kg,
 - Polarization block 2 kg; analyzer block 2 kg.

This is the first time the combined use of real-time spectroellipsometry measurements and data processing methods have been realized in an Adaptive Identifier (Fig. 1).

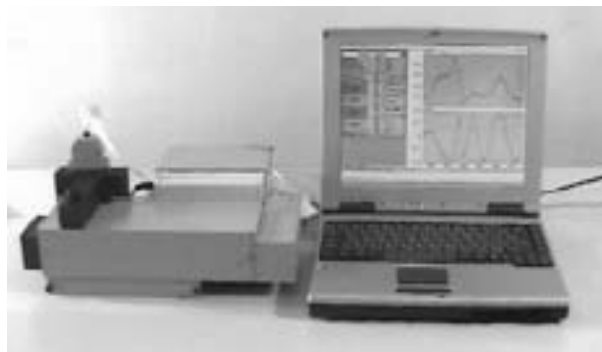


Fig. 1 High precision real-time multi-wavelengths spectroscopic ellipsometer with binary polarization modulation.

Adaptive Identifier device composition

- Polarizer block,
- Analyzer block,
- Power supply unit,
- Illuminator,
- Fiber-optic cable,
- Notebook with interface unit,
- Wide-band filters.

The algorithmic support of the Adaptive Identifier is based on a complex application of recognition and classification algorithms using 128 spectra images registered during a fixed period of time (Mkrtchyan *et al.*, 2004; Mkrtchyan *et al.*, 2005).

A time interval of 1 second is usually established and provides about 30 values of brightness for each of the 128 optical channels. The spectra obtained are sources for a set of statistical parameters and different characteristics united into vector spaces to be used for comparison with the standard samples of common pollutants stored on the computer.

The technology of this comparison depends on the diversity of identification methods. The system is trained to recognize the pollutants of an aquatic environment.

The Adaptive Identifier is designed to learn from the measurements of spectral characteristics and the simultaneous independent measurement of chemical element contents in the aquatic environment. As a result, a standard data bank is created in the knowledge base so that identifications and comparisons can be made. The software of the Adaptive Identifier provides different algorithms for the solution for identification problems, and cluster analysis is among of them.

Using spectroellipsometric technology:

1. Measurements of natural and waste water quality may be performed using:
 - a) A **transmission scheme** when quality of the sample is measured by inserting the fused quartz cuvette containing analyzed water into the spectroellipsometer device.
 - b) A **reflection scheme** when the quality of water is measured by inserting the spectroellipsometer sensor into water media being examined.
2. Because of the high accuracy of measurements with the spectroellipsometer, it is not possible to

use a whole method potential for remote measurements of natural and waste water quality. (Even small waves, ripples, foam can influence the quality of measurements.)

Results

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 pollution in the atmosphere and the estimation of the conditions of other elements in the environment whose spectral images may change.

An adaptive spectroellipsometric technology may be applied to the following areas for:

- Estimation of natural and wastewater quality,
- Analysis of liquids in medicine, biochemistry, food industry,
- Measurement of the mineralization level and chemical pollution of reservoirs, depending on the pollution type,
- Estimation of water salinity variations,
- Ellipsometrically based biosensor and gas sensor systems,
- Testing organic pollution clots in the water environment.

Experience

The Adaptive Identifier was tested under expeditionary conditions on board the R/V *Dmitry Mendeleev* in the Japan Sea, in the central areas of the Pacific Ocean, and during the investigation of aqueous systems of South Vietnam and Siberia (Lake Baikal, Angara and Yenisey rivers) within the framework of Russian–American and Russian–Vietnamese ecological expeditions.

A Russian–Vietnamese scientific and engineering laboratory has been built to create a standards base

and to prepare the Adaptive Identifier for full-scale production.

Conclusions

The main objective of this work is to create compact information systems for monitoring the quality of the 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, using a combination 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, and has 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 modeling for:

- Creation of a new element base for polarization optics with simple and efficient switches of the polarization state (SPS) that will successfully substitute for the conventional expensive polarizer–modulators of polarization state with rotating polarization elements;
- Optimization of the ellipsometric method regarding the change of amplitudes and phases of mutually orthogonal components of electromagnetic radiation used to measure the thickness of thin films on a water surface, and the determination of sensitivity and precision limits of adaptive spectroellipsometers in different operating regimes;
- Creation of methods for investigating the water surface, and the 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 used for the measurement of pollution levels in the aquatic

environment to be employed for training the adaptive spectroellipsometer.

The **experimental part** of the work described in report will include a description of the laboratory and on-site measurements of absorption, scattering, and reflection of electromagnetic waves from different aquatic objects.

The results given in this paper illustrate how the combined use of spectroellipsometric measurements and recognition algorithms give a possibility to economize material resources. It is obvious that the strategy of the modeling technology is in the interplay of model calculations and on-site experiments.

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