

THE CONTROL SOFTWARE OF THE PORTABLE RAMAN SPECTROMETER

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Abstract: The paper contains a description of the control software of a portable Raman spectrometer which was built in the Department of Optoelectronics and Electronic Systems Faculty of Electronics, Telecommunications and Informatics Gdansk University of Technology. The software has modular structure, which includes the laser control module and the spectrum acquisition module (laser power selection, working mode and data acquisition time) was described. The module of Raman spectra pre-processing (smoothing, background removal, normalization) was described in detail, with particular emphasis on its ergonomic use. The software was prepared for two different user types (experienced and inexperienced), allowing use by the advanced operator or by the less experienced personnel. The Raman spectra database with updating ability by external databases was presented, together with the selected identification algorithms.

Keywords: Raman Spectroscopy, identification

1. INTRODUCTION

Portable Raman spectrometers use dedicated software which controls the measurement process and performs necessary spectra processing in order to detect the investigated chemical samples. For this reason, the software quality is at least as important as the quality of the system hardware (laser, Raman probe, etc.). Moreover, the control software is the interface between the user and the device. Therefore, the ergonomic rules should ensure intuitive and convenient use of the device. This paper presents all modules of the software which controls the portable Raman spectrometer.

2. SOFTWARE STRUCTURE

The software was implemented in a form of a five modules which realize various functional blocks (Figure 1). The software works under control of Windows XP Embedded operating system, as a separate program prepared within the LabWindows/CVI integrated development environment. An important feature of the chosen development environment is availability of a comprehensive collection of the ready-made library functions, useful for data processing (e.g. filtering signals) and communication

between the hardware block via USB and RS-232 interface. These libraries considerably simplified the process of software development.

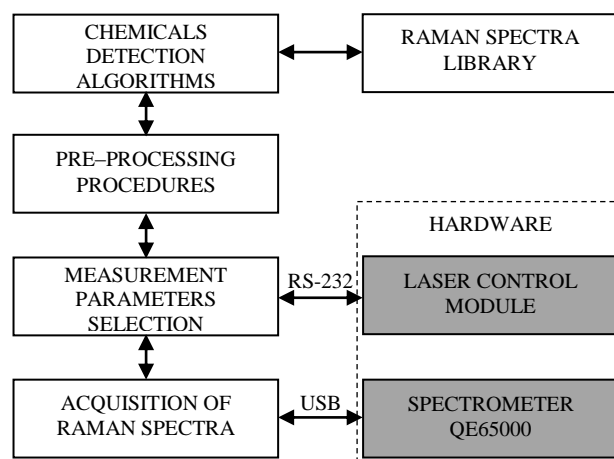


Fig. 1. Modular structure of the prepared control software

The block of Measurement Parameters Selection (Fig.1) performs a role of the user interface for the whole application and controls, through the RS-232 interface, the hardware used to control the two excitation lasers (785 nm and 355 nm) simultaneously. This block allows a selection of data acquisition time and temperature of the applied CCD detector, which is associated with noise intensity presented in the recorded spectrum. It also allows a choice of the measurement mode (synchronous or continuous) and power of the excitation laser beam. In the case of synchronous measurement it is possible to select a type of laser beam modulation and its frequency (Fig. 2).

Another part of software is the Acquisition of Raman Spectra module. This module requires a driver prepared by OceanOptics for National Instruments LabWindows/CVI integrated development environment. Transmission between the spectrometers and the acquisition module is done via USB interface.



Fig. 2. User interface of the prepared software (Measurement Parameters Selection module)

The next task of the control software, in addition to control the measurement process, is to carry out pre-processing procedures of the registered spectrum (Pre-Processing Procedures Block, Fig 1). This module allows to remove the spectrum background, spectrum smoothing and reduction of the etaloning effect (Fig. 3) [1,2]. It allows reduction of the investigated sample packaging for its detection efficiency [3].

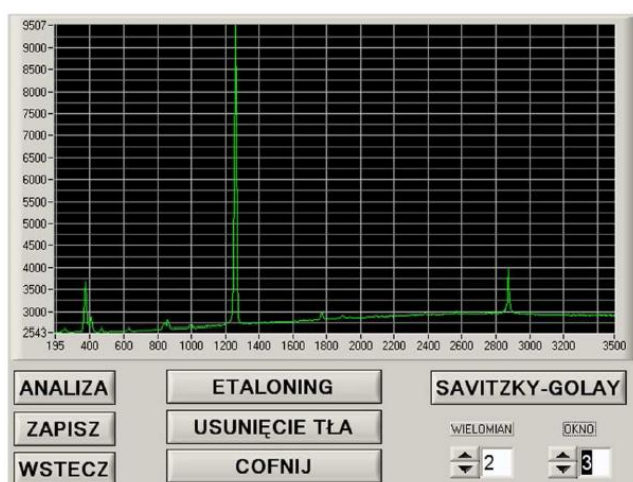


Fig. 3. User interface of the module Pre-Processing Procedures

All the modules were designed to make as easy as possible the use of control software by a small touch LCD screen. Therefore, all the buttons are of such size which enables their use by pressing by index finger. The user interface uses very legible fonts of sufficient size.

3. THE APPLIED DETECTION ALGORITHMS

For highly-efficient detection of the chemicals the module Chemicals Detection Algorithms (Fig. 1) was prepared. Detection of the investigated chemicals is done by comparing the measured Raman spectrum with each spectrum from the Raman Spectra Library and indicating which spectrum is the most similar to the measured one. This module allows chemicals identification in two modes. The first mode is the Full Spectrum Matching Methods. The second one is called the Peak Matching Methods (Fig. 4) [4].

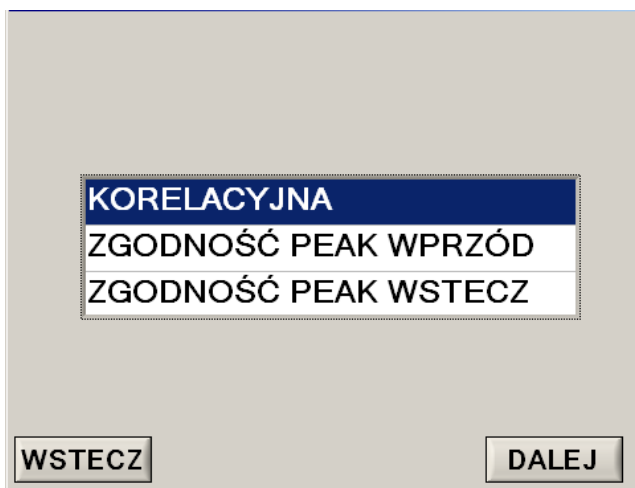


Fig. 4. The window for detection algorithm selection; the algorithms are included within the module Chemicals Detection Algorithms

In the Full Spectrum Matching Methods (called also correlation methods), the spectra comparison is done by calculating the values of all the corresponding spectra samples (or their first derivatives) of the measured spectrum with the spectrum from the database according to the preset norms (e.g. absolute value of difference, squared difference) [2,4]. The final value returned by these algorithms is a number (usually within the range 0÷100) that specifies a degree of similarity between the compared spectra (Fig. 5). High value of that number means high similarity between two compared spectra.

	NAZWA	ZGODNOŚĆ [%]
1	Cykloheksan	98,19
2	iso-Butanol	5,51
3	Cellulose Nitrate	5,14
4	2 Nitrotoluene	5,11
5	Sodium Peroxide	4,18

Buttons: WSTECZ, PORÓWNAJ, DALEJ

Fig. 5. Results of detection algorithm using correlation methods

The correlation methods may fail when the recorded spectra are noisy or have some background. In this case the Peak Matching method can be more effective.

In the Peak Matching Methods the selected parameters (position and relative amplitude) of the spectral lines are compared only. By analyzing the differences in position and relative amplitudes of these spectral lines, each spectral line gets a score (0÷100). The total score is calculated by summing up the results for all individual spectral lines and normalized by the normalizing factor to obtain the final value in the range 0÷100, as in the case of correlation methods. The estimated value responds to the number of detected spectral lines in the measured spectrum (Forward Peak Search) or the number of spectral lines detected in the identified database record (Reverse Peak Search) [4].

It should be underlined that the Forward Peak Search algorithm detects the spectrum from the database which has all the spectral lines present in the measured spectrum. This algorithm cannot detect chemical components when the investigated sample is a mixture of a few different chemicals.

The Reverse Peak Search algorithm is not sensitive to the presence in the measured spectrum of more spectral lines than in the spectrum of the identified database record. This means that in the case of chemical mixtures (presence of spectral lines caused by different compounds), the algorithm will be able to detect all separate compounds. This seems to be particularly useful for identification of various components from the data base and present in the examined mixture. It should be noted that this algorithm may indicate false chemical detection when only one or at most a few spectral lines are close to the location of the spectral lines present in the measured spectrum.

4. THE CONCEPT OF TWO DIFFERENT TYPES OF DEVICE OPERATORS

At an early stage of the design process of the portable Raman spectrometer, it was assumed that it will be operated by two groups of operators. The first group are the experienced users, the second are operators, who do not have expertise in chemistry and physics. A selection of the operator type occurs by logging into the control software after switching on the device. The act of entering a valid username and password (Fig.6) switches automatically the control software to the appropriate operator type.

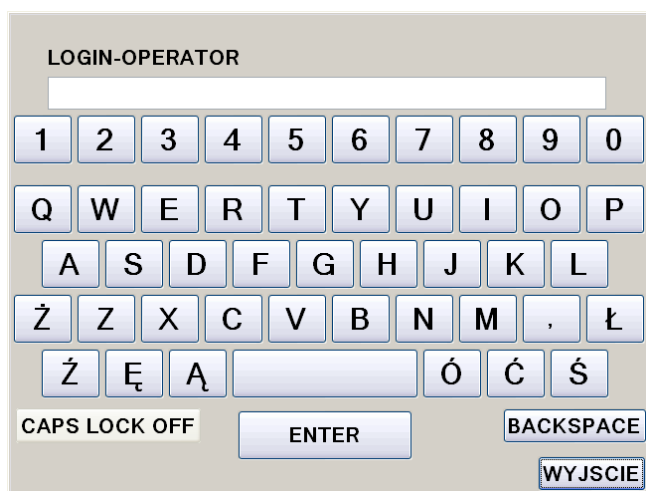


Fig. 6. The login window into the control software

In experienced mode an operator has access to the settings of various functions (acquisition time, the CCD temperature, data acquisition modes, laser power) and can control manually parameters of pre-processing procedures of Raman spectra. That operator type also has the complete access to the spectra collected in the built-in Raman spectra library. This means that it can freely browse and add to the spectral library the measured spectra of various substances which have not been present in the database.

Inexperienced operator has limited access to the device functions. In his case, the most of the Raman spectrum processing operations are done automatically. The pre-processing procedure is done without operator intervention (the parameters are setup up automatically). In this mode, the menu is simplified as well. The user only has access to the

most relevant information about the measurement process. The access to the built-in Raman spectra library is limited to read-only functionality.

The created user profiles help to operate the device more easily by persons who don't need to know too many features of the Raman spectrometer.

5. RAMAN SPECTRA LIBRARY

The detection process of chemical substances by measuring the Raman spectrum is done by comparing the recorded spectrum with the spectra stored in the database (Fig. 7).

	NAZWA	KOLOR	CZAS_POMIARU	LASER	OPERATOR	DATA
104	Dichloro-ethylene		70,0	785nm		08-08-20
105	Dieldrin		80,0	785nm		08-08-20
106	Dodecane		50,0	785nm		08-08-20
107	Ephedrine Hydrochl		100,0	785nm		08-08-20
108	Ethanol		120,0	785nm		08-08-20
109	Ether		40,0	785nm		08-08-20
110	Ethyl Acetate		30,0	785nm		08-08-20
111	Ethylene Glycol		180,0	785nm		08-08-20
112	Fenfluramine HCl		150,0	785nm		08-08-20
113	Fentanyl Citrate		400,0	785nm		08-08-20
114	Fluoxetine HCl		600,0	785nm		08-08-20
115	Flurazepam 2HCl		200,0	785nm		08-08-20

Buttons: POKAŻ, POKAŻ KOMPONENTY, ZAPIS SPC, WSTECZ, POKAŻ SZCZEGÓŁY, ODCZYT SPC

Fig. 7. The window listing the components of the built-in Raman Spectra library

The appropriate structure of the database is crucial from the point of view of the collected Raman spectra management, and the speed of chemical detection algorithms. In practice, different database structures can be used, starting from a very simple data stored in the text files to the complex database systems using e.g. an SQL engine. The use of more advanced database systems relieves the user from the detailed data management within the database. These systems control data integrity and can validate data entries. However, this solution requires additional software thread working at the same time as the main application. Thus, some additional CPU-intensive processes, can increase demand for electricity and computing. This is very disadvantageous for a portable device having limited power source. Therefore, the designed portable device implemented a dedicated database having the data structures saved in a few separate ASCII files (Fig. 8).

The table SPECTRUM stores information about the chemicals (physical state, color, smell, etc.), conditions of their Raman spectra measurements (exposure time, wavelength of the excitation laser, temperature of the detector, etc.) and data describing the registered spectra (number of points of the spectrum, Raman shift range, amplitude and position of the strongest spectral lines). It is assumed that the investigated chemicals may consist of ten components in maximum. This fact is marked by the dotted line on the figure 8.

The table SPEKTRUM_DANE stores two vectors corresponding to the X and Y coordinates of points belonging to the spectrum. The tables KOMPONENTY, SUBSTANCJE and STRUCT_KOMP collect information about the components of the investigate samples.

Information about name, common name, serial numbers, descriptions of the manufacturer, CAS number (unique number given by Chemical Abstracts Service organization), IUPAC name (name recommended by the International Union of Pure and Applied Chemistry), can be included there.

In order to reduce the database volume, the fields stanskup, kolor, zapach in the SPECTRUM table and the field wytwórca in the KOMPONENTY table have been indexed. This means that these fields don't contain the pure data, but there are the number (id_skupienie, id_zapach, id_kolor, id_wytworcy), which clearly describe the selected substance features.

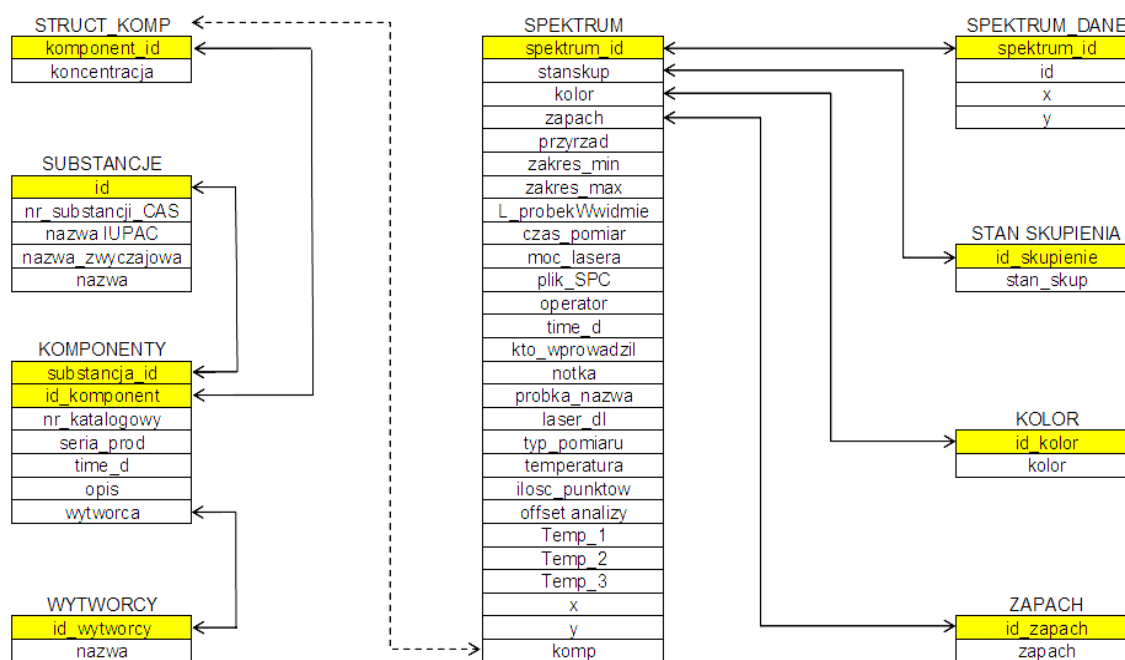


Fig. 8. The structure of the implemented database

6. SUMMARY

The concept of the software which control measurements done by the portable Raman spectrometer was presented. Additionally, some algorithms used for spectra pre-processing and detection were also described.

The prepared software was prepared using LabWindows/CVI environment. The choice of the software environment was determined by ability of producing an installation version and mathematical libraries used in pre-processing and detection functions. The installation version of the created application takes about 40 MB of disk space.

The efficiency of the built-in database, which takes about 8 MB of the disk space, was positively tested for approximately 240 records. We can expect that the prepared software should work effectively with the Raman spectra database at least up to a few thousands of Raman spectra.

7. BIBLIOGRAPHY

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OPROGRAMOWANIE STERUJĄCE PRZENOŚNYM SPEKTROMETREM RAMANA

Słowa kluczowe: Spektroskopia Ramana, Identyfikacja

Praca zawiera opis oprogramowania sterującego przenośnym spektrometrem Ramana, który został zbudowany w Katedrze Optoelektroniki i Systemów Elektronicznych Wydziału Elektroniki, Telekomunikacji i Informatyki Politechniki Gdańskiej, w trakcie realizacji grantu rozwojowego. Opisano modułową budowę oprogramowania, zawierającego moduł sterujący pracą laserów oraz procesem akwizycji widma. Bardziej szczegółowo przedstawiono moduły realizujące funkcje wstępnego przetwarzania widm Ramana, ze szczególnym uwzględnieniem ergonomii korzystania z urządzenia w warunkach pomiarów w terenie. Oprogramowanie zrealizowano w koncepcji dwóch użytkowników (zaawansowany i podstawowy), umożliwiając tym samym obsługę urządzenia przez doświadczonych operatorów oraz przez personel o ograniczonych kwalifikacjach. Przedstawiono także budowę bazy danych widm Ramana. Scharakteryzowano również algorytmy dokonujące identyfikacji widm.