Science and Innovation. 2014. V. 10. No. 2. P. 72—75

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APPLICATION OF PORTABLE RAMAN SPECTROMETERS FOR RAPID PRODUCTION CONTROL AND ANALYSIS IN THE FIELD ENVIRONMENT

The fundamental theory of Raman spectroscopy and its application in various fields have been described. Thermo Fisher Scientific Corporation, a world leader in high-tech instruments, has designed a series of portable Raman spectrometers for a broad scope of application.

Key words: Raman spectroscopy, Fourier transform infrared spectroscopy, near-infrared spectroscopy, portable spectrometers, identification, and TruScan.

The group of analytical methods known as *vibrational* spectroscopy includes three basic techniques, namely the Fourier transform infrared (FTIR), the near infrared (NIR), and the Raman spectroscopy. Each of them has its advantages and disadvantages. Historically, the FT-IR spectroscopy is considered to be a working method for the laboratory analysis of raw materials. This method has a high molecular selectivity and gives reliable results. However, due to the design features of currently available IR spectrometers and the complications associated with the selection and preparation of samples, the analysis of raw materials is made in the laboratory environment only. The necessity to monitor the physical conditions of certain raw materials and to carry out the laboratory analysis at the point of sampling has stimulated the development and use of portable NIR spectrometers. Despite a worse selectivity and impact on the measured value of sample physical characteristics (such as particle size, packing density, and moisture content) the NIR spectroscopy is of considerable interest. The Raman spectroscopy which combines many advantages of FTIR and NIF spectroscopy has become available thanks to a recent progress in enhancing sensitivity, miniaturization, and integrated functions of data analysis. Thus, today, high selectivity, rapidity of analysis, and portability of modern Raman spectrometers allow the researchers to identify raw materials directly in the place where it is necessary.

The Raman spectroscopy is a type of vibrational spectroscopy used to study the molecular structure of matter in the liquid, gas, and solid state, as well as in the state of powder, gel, slurries, and aqueous solutions. The method is based on the effect discovered in 1928, by Raman, an Indian physicist, and named after him. The Raman effect is the inelastic scattering of optical radiation on the molecules of matter, which is accompanied by a noticeable change in its frequency. In contrast to the Rayleigh scattering, in case of Raman scattered radiation, in the spectrum

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there appear new spectral lines which are absent in the spectrum of primary (exciting) radiation. The number and location of new lines are determined by the matter chemical composition and molecular structure. So, each agent has a unique Raman spectrum that can be used for its identification.

The mechanism of Raman scattering differs from the mechanism of FTIR or NIR absorption. The IR and Raman spectra complement each other instead of overlapping, since they are determined by different rules of origin. Using these methods in combination the researchers can get maximum information about the matter vibrational and rotational spectra.

One of the biggest advantages of Raman spectroscopy as compared with other technologies is the ease of sampling and the absence of sample preparation. Glass, plastic sheeting, and water have a very weak Raman scattering, which allows the researchers to carry out the measurements directly through the walls of containers and packaging (e.g. UV cuvettes, test tubes for NMR, capillary tubes, vials, plastic bags or bottles) unsuitable for the IR spectroscopy. Thus, the sample analysis using the Raman spectroscopy is a non-contact and non-destructive one. It is possible to get the Raman spectrum of aqueous solutions since water is ignored for the purpose of analysis and does not preclude the analysis of solved substance. Another advantage of the Raman spectroscopy over the NIR spectroscopy is its validity regardless of the physical state of sample. This results in a much simpler approach to the spectral data interpretation. The procedures for obtaining and analyzing the Raman spectra can be performed using the Raman libraries, inasmuch as the peaks are sufficiently clear and sharp and do not shift in case of deviations in the sample physical state, except for effect of certain chemical groups.

The limitation for obtaining the Raman spectra is fluorescence that occurs when the excited molecule's electrons, when returning to the state of rest, release excessive energy by issuing photons. The fluorescence manifests itself in the Raman spectrum as a high background signal which in some cases can be quite intensive and overlap the Raman signal. In the most cases, this effect is avoided by the use of lasers with a wavelength of 785 nm (or more) as a source of exciting radiation.

In the past, the Raman spectroscopy was not as popular as the infrared spectroscopy, and was often used in research laboratories only. The laser devices were big, unreliable, and expensive. They required very complicated maintenance. In addition, the sensitivity of these devices was very low, so every sample measurement lasted several hours. Thanks to the development of Raman spectroscopy with Fourier transform (FT-Raman) the situation improved in the late 1980s – the early 1990s. The next step was to develop high-performance optical blocking filters, as well as cheaper and more sensitive CCD-matrices (Charge Coupled Devices, CCD) at the beginning and in the middle of the 1990s. Since that time, the Raman spectroscopy started to get used as a routine laboratory method. However, the instruments developed using these achievements remained large, quite expensive, and suitable only for the use in controlled laboratory conditions.

Further progress in the field of semiconductor lasers, optical miniaturization technologies, compact data processing devices, and algorithms of probabilistic and statistical analysis has allowed the engineers to develop a compact, reliable, autonomous, and portable Raman spectrometer that can be used even under harsh conditions outside the laboratory.

APPLICATION OF THE RAMAN SPECTROSCOPY

The Raman spectroscopy is used in many fields of science and technologies where it is necessary to conduct non-destructive chemical analysis and visualization. Both in chemistry and biology the Raman spectroscopy is used to identify chemical compounds for determining their functional groups and conformations of complex molecules. It can be used for rapid characterization of chemical composition and structure of samples regardless of their physical conditions. Due to a high sensitivity of modern Raman spectrometers the

collection of information in a matter of seconds has become commonplace, since in the recent years the method has got increasingly important in the industries that require rapid identification of unknown compounds. The reason for this interest in Raman spectrometers is the fact that these spectrometers are equipped with intelligent software which can make decisions and are ready to be used by spectral libraries. These devices are an ideal tool for obtaining «molecular fingerprints».

In contrast to the traditional analytical methods, such as high-performance liquid chromatography (HPLC), FTIR, and NIR spectroscopy which are more time-consuming and often require the specific procedures for sample preparation, the Raman spectrometers can be used in the field and operating conditions insofar as they practically require neither any sample preparation nor direct contact with samples. They can make analysis directly through transparent packaging material such as glass or plastic.

The scope of the Raman spectroscopy application includes:

- Forensic examination;
- Forensics and security;
- Pharmaceutical industry;
- Agriculture and food security;
- Identification of raw materials in the course of incoming inspection; and
- Identification of counterfeit products.

Some of the above spheres have been included in this list due to the development of modern high-performance, portable, and hand-held Raman spectrometers which are fast, more reliable, and cheaper due to the miniaturized components. In particular, the reduction of spectrometer size allows the researchers to use it outside laboratories, in new areas where previously it was impossible because of the instrument awkwardness.

Thermo Fisher Scientific, a world-renowned manufacturer of high-tech analytical equipment, recognizes the need for reliable portable instruments and has developed a series of small-sized Raman spectrometers which are extremely easy to use and require minimal involvement of users in the creation of methods and interpretation of results. The approach to data analysis used in the *TruScan* spectrometers and based on patented algorithm of probabilistic-statistical analysis is the most reliable one and allows us to quickly implement new methods without any decrease in speed and accuracy in the course of routine use.

Among the examples of successful application of Raman spectroscopy there are identification of unknown substances, analysis of raw materials, as well as qualitative and quantitative analysis of finished products in pharmaceutical industry [1, 2]. The *TruScan* RM™ Raman spectrometer manufactured by *Thermo Scientific* is a portable analyzer specially designed for the use in pharmaceutical manufacturing, rapid identification of chemical compounds, quick examination of chemical composition authenticity and for control of counterfeit drugs.

Also, the Raman spectroscopy is widely used in forensic analysis of drugs, explosives, and other dangerous substances. To address these challenges *Thermo Scientific* has developed *TruNarc*™, a specialized analyzer which is a portable Raman spectrometer for rapid identification of suspected substances outside the laboratory, without direct contact with majority of samples. It is a lightweight and easy to use spectrometer providing the fast and accurate analysis of samples in any place where it is necessary.

CONCLUSIONS

The Raman spectroscopy is a powerful analytical tool with many advantages. The method is easy to use, inasmuch as it virtually does not require any sample preparation. The resultant spectral information can be used for both identification and quantitative analysis.

The recent achievements in the production of radiation sources and detectors based on progress in user interface design, sampling and data processing algorithms allow the engineers to create portable Raman spectrometers which make it possible not only to conduct laboratory research, but also to use them for chemometrics by experienced highly qualified staff.

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ИСПОЛЬЗОВАНИЕ ПОРТАТИВНЫХ РАМАНОВСКИХ СПЕКТРОМЕТРОВ ДЛЯ ЭКСПРЕСС-КОНТРОЛЯ ПРОИЗВОДСТВЕННЫХ ПРОЦЕССОВ И АНАЛИЗА В ПОЛЕВЫХ УСЛОВИЯХ

Описаны основы метода рамановской спектроскопии, а также ключевые области использования портативных спектрометров. Компания Thermo Fisher Scientific, всемирно известный производитель высокотехнологического аналитического оборудования, разработала серию портативных рамановских спектрометров.

Ключевые слова: рамановская спектроскопия, ИК-Фурье спектроскопия, БлИК-спектроскопия, портативные спектрометры, идентификация, TruScan.

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ВИКОРИСТАННЯ ПОРТАТИВНИХ РАМАНІВСЬКИХ СПЕКТРОМЕТРІВ ДЛЯ ЕКСПРЕС-КОНТРОЛЮ ВИРОБНИЧИХ ПРОЦЕСІВ ТА АНАЛІЗУ У ПОЛЬОВИХ УМОВАХ

Описано основи методу раманівської спектроскопії, а також ключові області використання портативних спектрометрів. Компанія Thermo Fisher Scientific, всесвітньо відомий виробник високотехнологічного аналітичного обладнання, розробила серію портативних раманівських спектрометрів.

Ключові слова: раманівська спектроскопія, ІЧ-Фур'є спектроскопія, БлІЧ-спектроскопія, портативні спектрометри, ідентифікація, TruScan.

Received 25.12.13