In Celebration of the 50th Anniversary of the
SOCIETY FOR APPLIED SPECTROSCOPY
A Selection of Ground-Breaking Papers from
Applied Spectroscopy

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A Selection of Ground-Breaking Papers from Applied Spectroscopy
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Inductively Coupled Plasma-Atomic Emission Spectroscopy: Prominent Lines

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The prominent lines of 78 elements as emitted in an inductively coupled plasma excitation source have been identified. The lines are listed alphabetically by element and numerically by wavelength. Detection limit capabilities are estimated for each spectral line.

Volume 31, Number 3, 1979, pp. 256 - 271
372 citations

Double Resonance Excitation of Fluorescence in the Condensed Phase—An Alternative to Infrared, Raman, and Fluorescence Spectroscopy

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The feasibility of performing a double resonance excitation of fluorescence from molecules in a condensed phase is discussed. A rotational excitation can be created by either stimulated Raman scattering or infrared absorption while a second excitation can create the molecule to an excited electronic state from which fluorescence can occur. By providing high rates of excitation, one can overcome the rapid vibrational relaxation rates to produce fluorescence. By measuring the second excitation frequency in synchronism with either the infrared frequency or the difference frequency, producing the stimulated Raman scattering, one can obtain spectra that are analogous to Raman or infrared spectra. This approach would have the short lines characteristic of fluorescence spectroscopy.

Volume 34, Number 2, 1980, pp. 151 - 157
Meggers Award

Single-Atom Detection*

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An overview is presented of the principles and achievements of various laser-assisted detection techniques that have been developed to observe a single or a small number of neutral atoms in a plasma or gas discharge. The main emphasis is on the application of laser-induced fluorescence techniques and their significance for the improvement of analytical detection limits. Section I describes the general implications of these techniques and contains schematic representations for the mass and the relaxation of the signal. An intrinsic limit of detection is defined that relates to the statistical fluctuation of the number of registered atoms in the observation volume. Section II gives a classification and a more detailed description of reported techniques. Experimental detection limits are compared with the intrinsic limits predicted by theory. In Section III, conclusions are drawn about the state-of-the-art and suggestions are made for further improvements, including the lowering of the analytical detection limit.

Volume 35, Number 1, 1981, pp. 1 - 14
Meggers Award

Fourier Self-Deconvolution: A Method for Resolving Intrinsically Overlapped Bands*

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The general theory of Fourier self-deconvolution, i.e., spectral deconvolution in the form of Fourier transforms and the intrinsic line-shape, is delineated. The method provides a way of computationally resolving overlapped lines that can not be instrumentally resolved due to their intrinsic line width. Examples of the application of the technique to synthetic and experimental infrared spectra are presented, and potential applications are discussed. It is shown that lines in spectra having much stronger signals than weaker lines (≈1000) can readily be reduced in width by a factor of 3. The method is applicable to a variety of spectroscopic techniques.

Volume 35, Number 3, 1981, pp. 271 - 276
850 citations

A New Background-correction Method for Atomic Absorption Spectrometry

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A new method is described and tested for background correction in atomic absorption spectrometry. Applicable to flame or furnace atomizers, the method is capable of correcting backgrounds caused by molecular absorption, particulate scattering, and atomic-line overlap, even up to an absorbance value of 3. Like the Zeman approach, the new method applies its correction very near the atomic line of interest, can employ single-beam optics, and requires no auxiliary source. However, no auxiliary lamp or other costly peripherals are required and working curves are single-valued. The new technique is based on the broadening which occurs in a hollow-cathode optical line when the lamp is operated at high currents. Under such conditions, the absorbance measured at a narrow (atomic) line is low, whereas the apparent absorbance caused by a broad-band background contribution remains high as when the lamp is operated at conventional current levels. Background correction can therefore be effected by taking the difference in absorbance measured with the lamp operated at high and low currents. The new technique is evaluated in its ability to correct several different kinds of background interference and is critically compared with competitive methods.

Volume 37, Number 5, 1983, pp. 419 - 424
Meggers Award

Background Spectral Features in Inductively Coupled Plasma/Mass Spectrometry

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Basic background mass spectra of the inductively coupled plasma are presented in this report. The background spectral features were measured for the mass range 1 to 154 amu and for solutions of nitric acid, hydrochloric acid, and sulfuric acid. Background spectra are measured for all solutions for the mass range 1 to 154 amu and extensive tables are presented for observed species and their isotopic combinations.

Volume 40, Number 4, 1986, pp. 445 - 460
329 citations

FT-Raman Spectroscopy: Development and Justification

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There has long been a widespread interest in the feasibility of Fourier transform Raman spectroscopy. The well-developed techniques of FTR spectroscopy are particularly well suited for the vibrational excitation of molecules in solution. The approach would have the advantages of simplicity characteristic of Raman spectroscopy. The Raman spectrum is a fingerprint characteristic of the sample, and it is a very sensitive technique. This approach would have the advantage of simplicity characteristic of Raman spectroscopy.

Volume 40, Number 2, 1986, pp. 133 - 137
Meggers Award 272 citations

Standard Normal Variate Transformation and De-trending of Near-Infrared Diffuse Reflectance Spectra

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Particle size, scatter, and multi-colinearity are long-standing problems unsolved in diffuse reflectance spectrometry. Multiplicative combinations of these factors are the major factor inhibiting the interpretation of near-infrared diffuse reflectance spectra. Sample particle size accounts for the majority of the variance, while variance due to chemical composition is small. Procedures are presented whereby physical and chemical variance can be separated. Mathematical transformations—standard normal variate (SNV) and detrending (DT)—are applied to individual NIR diffuse reflectance spectra are presented. The standard normal variate approach effectively removes the multiplicative influence of particle size and particle size. De-trending, a technique for the variance baseline shift and a residual, generally found in the reflectance spectra of powdered or dusted samples, is used in a second-degree polynomial regression. NIR diffuse reflectance spectra transformed by these procedures can be used to predict the concentration of a specific component of the heterogeneous mixture. A demonstration of this technique is provided using the near-infrared diffuse reflectance spectra of a mixture of polystyrene and the proteinaceous component of human stratum corneum to demonstrate the utility of this technique.

Volume 43, Number 5, 1989, pp. 772 - 777
456 citations

Two-Dimensional Infrared (2D IR) Spectroscopy: Theory and Applications

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A novel concept in vibrational spectroscopy called two-dimensional infrared (2D IR) spectroscopy is described. In 2D IR, a spectrum defined by two independent wavenumbers is generated by a cross-correlation analysis of dynamic fluctuations of IR signals induced by an external perturbation. 2D IR spectra are especially suited for elucidating various chemical interactions among functional groups. Noticeable features of the 2D IR approach are: simplification of complex spectra consisting of many overlapped peaks; enhancement of spectral resolution by optimising peaks over the second dimension; and establishment of unambiguous assignments through correlation analysis of bands selectively excited by various interaction mechanisms. Procedures for generating 2D IR spectra are also described. The new procedure is illustrated for the analysis of polystyrene and the proteinaceous component of human stratum corneum to demonstrate the utility of this technique.

Volume 44, Number 4, 1990, pp. 550 - 561
335 citations

New Procedure for Quantitative Elemental Analysis by Laser-Induced Plasma Spectroscopy

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A new procedure, based on the laser-induced plasma spectroscopy (LIPS) technique, is proposed for calibration-free quantitative elemental analysis of materials. The method here presented, based on an algorithm developed and patented by IFAM-CNR, allows the detection and quantification of several elements, using low power and low cost equipment. The proposed method is applied to the determination of light elements (Bi, P, As, Se, S, Si, Mg, Na, K). The general applicability of the method is demonstrated by the analysis of the composition of metallic alloys and by quantitative determination of the composition of the air.

Volume 53, Number 8, 1999, pp. 960 - 964
83 citations

The Meggers Award has been given annually since 1960 to one article published in Applied Spectroscopy that is judged as the most outstanding.

The number of citations is from the Science Citation Index list of the papers in Applied Spectroscopy that have been cited most often.
Near-Infrared Acousto-optic Filtered Spectroscopic Microscopy: A Solid-State Approach to Chemical Imaging

PATRICK J. TREADO, IRA W. LEVIN, and E. NEIL LEWIS

A new instrumented approach for performing spectroscopic imaging microscopy is described. The instrument integrates an acousto-optic tunable filter (AOTF) and charge-coupled-device (CCD) detector with an infinity-corrected microscope for operation in the visible and near-infrared (NIR) spectral regions. Images at moderate spectral resolution (2 mm) and high spatial resolution (5 mm) can be collected rapidly. Data are presented containing 228 X 230 pixels, although images with significantly larger formats can be collected in approximately the same time. In operation, the CCD is used as a true imaging detector, while monochromatic light is provided by using the AOTF and quartz tungsten halogen lamp to create a variable source. The instrument is entirely solid state, containing no moving parts, and can be readily configured for both absorption and reflection spectroscopy. We present visible absorption spectra of human epithelial cells, as well as NIR reflection spectra of a bacterially phosphorylated suspension, to demonstrate the potential of the technique in the study of biological materials. Extensions and future applications of this work are discussed.

Volume 46, Number 4, 1992, pp. 553 - 559

Generalized Two-Dimensional Correlation Method Applicable to Infrared, Raman, and Other Types of Spectroscopy

I. NODA

A two-dimensional (2D) correlation method generally applicable to various types of spectroscopy, including IR and Raman spectroscopy, is introduced. In the proposed 2D correlation scheme, an internal perturbation is applied to a system while being monitored by an electromagnetic probe. With the application of a correlation analysis to spectra, intensity changes induced by the perturbation, new types of spectra defined by two independent spectral variable axes are obtained. Such a two-dimensional correlation spectra exhibit characteristic spectral features not readily discernible in conventional one-dimensional spectra. While a similar 2D correlation formula has already been developed in the past for analysis of simple sinusoidally varying IR signals, the newly proposed formulation is designed to handle signals fluctuating as an arbitrary function of time, or any other physical variable. This development makes the 2D correlation approach a valuable spectroscopic tool, generally applicable to a very wide range of applications. The basic property of 2D correlation spectra obtained by the new method is described first, and several practical aspects are analyzed by the proposed scheme to demonstrate the utility of generalized 2D correlation spectra. Potential applications of this 2D correlation approach are then explored.

Volume 47, Number 9, 1993, pp. 1329 - 1336

Efficient Rejection of Fluorescence from Raman Spectra Using Picosecond Kerr Gating

P. MATOUSEK,* M. TOWRIE, A. STANLEY, and A. W. PARKER

An efficient method for the rejection of fluorescence from picosecond time-resolved resonance Raman (ps-TRR) spectra, applicable also to ground-state Raman spectroscopy, has been demonstrated. The technique removes fluorescence from Raman light in the true domain using a Kerr gate driven by 110 ns., 3 ps, pulses at 800 nm and a repetition rate of 6.6 kHz, giving a response time of 5 ps, representing the highest time resolution achieved experimentally for rejecting fluorescence from Raman spectra. The effectiveness of the method is proven by measuring Raman solvent bands and ps-TRR spectra of $S_1$ quaterphenyl from solutions contaminated with the laser dye DCM using laser wavelengths which excite the dye and so produce intense fluorescence emission. The optical transmittances accounting for losses in the optical arrangement and fluorescence due to incoherent polarization remain in the Kerr medium in the open and closed modes were 1% and 0.005%, respectively. The use of the gate in a true-domain picosecond fluorescence measurement of DMABN is also demonstrated.

Volume 52, Number 12, 1999, pp. 1485 - 1489

Picosopic Time-Resolved Raman Spectroscopy of Solids: Capabilities and Limitations for Fluorescence Rejection and the Influence of Diffuse Reflectance

NEIL EVERALL,* THOMAS HARN, PAVEL MATOUSEK, ANTHONY W. PARKER, and MICHAEL TOWRIE

It has been known for many years that it should be possible to discriminate between Raman and fluorescence phenomena on the basis of their differing temporal responses. However, it is only relatively recently that optical technology has advanced sufficiently to achieve the necessary combination of high repetition rate and picosecond laser pulse coupled with "quartzic" multichannel detectors with matched repetition rates and short on-times. Both electronic and optical gating techniques have been shown to significantly improve the Raman spectra of highly fluorescent solids. However, the performance of such systems with solid materials has not been reported in detail. To partially redress this imbalance, this paper describes a picosecond time-resolved Raman spectroscopy of solids and powders. Excellent temporal resolution and fluorescence rejection was obtained with homogeneous films, but with powders, multiple scattering has permitted significant blurring of the time resolution. For instance, after excitation of a 1 ps pulse on a powdared sample of trans-stilbene, the Rayleigh signal was spread over 100 ps in time and the Raman signal persisted for more than 300 ps. Simple models are presented for predicting these temporal responses on the assumption that photons randomly "diffuse" through the powder, scattering at particle boundaries and sometimes re-emerging to be detected at a later time. These dynamics imply that fluorescence rejection with bulk powders might be less effective than with homogeneous solids as the broadened Raman signal would be incorrectly captured within the short detector "on" period. The fluorescence would be rejected, but so would the Raman signal (in some extent), giving a poor signal-to-noise ratio. This long-time signal persistence could also complicate the interpretation of pump-probe spectroscopy studies. However, further work is needed to assess the practical implications of these findings.

Volume 55, Number 12, 2001, pp. 1710 - 1717

Generalized Implementation of Rapid-Scan Fourier Transform Infrared Spectroscopic Imaging

SCOTT W. HUFFMAN, ROHIT BHARGAVA, and IRA W. LEVIN

We describe a novel, generalized data acquisition sequence to allow rapid-scan Fourier transform infrared (FT-IR) spectroscopic imaging using fixed focal array (FFA) detectors. This technique derives its flexibility from the reproducibility of modern FT-IR instrumentation and the availability of FFAs with simultaneous, full- band-through capabilities. Instead of scanning the entire interferogram in one mirror sweep over a predetermined range, as in traditional transmissive-modulation techniques, the monochromatic light from the interferometer is recorded over several mirror sweeps. The FFA detector is driven by a computer-specified delay with respect to the initiation of the mirror motion to provide a highly angular-sampled interferogram. By incorporating appropriate delays in subsequent interferometer mirror scans, the entire interferogram is sampled and reconstructed. The signal-to-noise ratio (SNR) of the resulting interferograms is analyzed and compared with step-scan spectroscopic imaging data.

Volume 56, Number 8, 2002, pp. 965 - 969

Numerical Simulations of Subsurface Probing in Diffusely Scattering Media Using Spatially Offset Raman Spectroscopy

P. MATOUSEK,* M. D. MORRIS, N. EVERALL, I. P. CLARK, M. TOWRIE, E. DRAPER, A. GOODSHIP, and A. W. PARKER

We present the first elementary model predicting how Raman intensities vary for a range of experimental variables for spatially offset Raman spectroscopy (SORS), a recently proposed technique for the effective removal of Raman spectra from diffuse layers in diffusely scattering media. The model was able to reproduce the key observations made from the first SORS experiments, namely the dependence of Raman signal intensity on optical effects such as the dilution and collection properties of spatial offsets and the interference between the offset layer and sub-layer. The application of the SORS concept to a three-layer system is also discussed. The model also clarifies that an anisotropic geometry, rather than a point-collection, would yield much improved data.

Volume 59, Number 12, 2005, pp. 1488 - 1492

In mid-1945, as World War II neared its end, a group of scientists in and around New York City formed a new organization, called The Society for Applied Spectroscopy. They also began a publication, The Society for Applied Spectroscopy Bulletin. There were some technical articles in it, and they were tutorial in nature. Over the next few years the Bulletin became a scientific journal, renamed Applied Spectroscopy. When a national spectroscopic society was formed in 1957, the New York group donated its name and the publication to the national organization, and became the New York Section. The cover of the January 1996 issue marked the 50th anniversary of Applied Spectroscopy. The upper left inset shows the cover of an early issue of the Bulletin. The cover of the journal in 1959 is shown on the top right. The national society assumed publication of the journal in 1960. The middle image shows the cover three years later, unchanged but for a new logo. The other images are photos of six of the people during the first fifty years. Two of them, John Ferraro and Leopold May, also served terms as President of SAS.