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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with
Bruce Chase, Peter Griffiths
and Joel Harris

A Selection of Ground-Breaking Papers from *Applied Spectroscopy* Chosen by Leopold May, Bruce Chase, Peter Griffiths and Joel Harris

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Inductively Coupled Plasma-Atomic Emission Spectroscopy: Prominent Lines

R. K. WINGE, V. J. PETERSON, and V. A. FASSEL
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The prominent lines of 70 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 33, Number 3, 1979, pp. 206 - 219
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 vibrational excitation can be created by either stimulated Raman scattering or infrared absorption while a second excitation can excite 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 scanning the second excitation frequency in synchronization 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 sharp 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 the gaseous state. Possible applications of these single-atom detection (SAD) techniques and their significance for the improvement of analytical detection limits are mentioned. Section I describes the general implications of SAD techniques and contains statistical expressions for the mean and the fluctuation 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*

JYRKI K. KAUPPINEN,† DOUGLAS J. MOFFATT, HENRY H. MANTSCH, and DAVID G. CAMERON
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The general theory of Fourier self-deconvolution, i.e., spectral deconvolution using Fourier transforms and the intrinsic line-shape, is developed. 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 moderate signal/noise ratios (~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 Zeeman 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 ancillary magnet 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 spectral line when the lamp is operated at high currents. Under such conditions, the absorbance measured for a narrow (atomic) line is low, whereas the apparent absorbance caused by a broad-band background contributor remains as high as when the lamp is operated at conventional current levels. Background correction can therefore be effected by taking the difference in absorbance's 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 nebulization of water and for 5% solutions of nitric acid, hydrochloric acid, and sulfuric acid. Background spectra are presented for all these solutions for the mass range 1 to 84 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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and Central Research Dept., Du Pont Experimental Station, Wilmington, Delaware (B.C.)

There has long been a widespread interest in the feasibility of Fourier transform Raman spectroscopy. The well-deserved reputation of FT-IR has generated hopes for similar benefits in Raman spectroscopy, and the complementarity of IR and Raman spectroscopy has made the use of a single instrument for both spectroscopies both convenient and cost-effective.

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-collinearity are long-standing problems encountered in diffuse reflectance spectrometry. Multiplicative combinations of these effects 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 de-trending (DT)--applicable to individual NIR diffuse reflectance spectra are presented. The standard normal variate approach effectively removes the multiplicative interferences of scatter and particle size. De-trending .accounts for the variation in base-line shift and curvilinearity, generally found in the reflectance spectra of powdered or densely packed samples, with the use of a second-degree polynomial regression. NIR diffuse reflectance spectra transposed by these methods are free from multi-collinearity and are not confused by the complexity of shape encountered with the use of derivative spectroscopy.

Volume 43, Number 5. 1989, pp. 772 - 777
488 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. Notable features of the 2D IR approach are: simplification of complex spectra consisting of many overlapped peaks; enhancement of spectral resolution by spreading peaks over the second dimension; and establishment of unambiguous assignments through correlation analysis of bands selectively coupled by various interaction mechanisms. The procedure for generating 2D IR correlation spectra and the properties of the 2D spectra are discussed in detail. Examples of 2D IR spectra are presented for atactic polystyrene and the proteinacious component of human stratum corneum to demonstrate the utility of this technique.

Volume 44, Number 4, 1990, pp. 550 -561
Meggers Award 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 matrix effects to be overcome, yielding precise and accurate quantitative results on elemental composition of materials without use of calibration curves. Some applications of the method are illustrated, for quantitative analysis of the composition of metallic alloys and quantitative determination of the composition of the atmosphere.

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

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A new instrumental 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 nm) and high spatial resolution (1 /zm) can be collected rapidly. Data are presented containing 128 x 128 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 wavelength selectivity is provided by using the AOTF and quartz tungsten halogen lamp to create a tunable source. The instrument is entirely solid state, containing no moving parts, and can be readily configured for both absorption and reflectance spectroscopies. We present visible absorption spectral images of human epithelial cells, as well as NIR vibrational absorption images of a hydrated phospholipid 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
Meggers Award

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

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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 external perturbation is applied to a system while being monitored by an electromagnetic probe. With the application of a correlation analysis to spectral intensity fluctuations induced by the perturbation, new types of spectra defined by two independent spectral variable axes are obtained. Such two-dimensional correlation spectra emphasize spectral features not readily observable in conventional one-dimensional spectra. While a similar 2D correlation formalism has already been developed in the past for analysis of simple sinusoidally varying IR signals, the newly proposed formalism 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 universal 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 spectral data sets 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
539 citations

Efficient Rejection of Fluorescence from Raman Spectra Using Picosecond Kerr Gating

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An efficient method for the rejection of fluorescence from picosecond time-resolved resonance Raman (ps-TR3) spectra, applicable also to ground-state Raman spectroscopy, has been demonstrated. The technique removes fluorescence from Raman light in the time domain using a Kerr gate driven by 110 mJ, 1 ps pulses at 800 nm and a repetition rate of 0.65 kHz, giving a response time of 3 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-TR3 spectra of S1 *p*-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 elements and losses due to incomplete polarization rotation in the Kerr medium in the open and closed states were 15% and 0.005%, respectively. The use of the gate in a time-resolved fluorescence measurement of DMABN is also demonstrated.

Volume 53, Number 12, 1999, pp. 1485 - 1489

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

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ICI PLC, Wilton Research Centre, Wilton, Redcar, Cleveland, TS10 4RF, UK (N.E.); National Starch and Chemical, 10 Finderne Avenue, Bridgewater, New Jersey (T.H.); and Central Laser Facility, CLRC Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire, OX1 0QX, UK (P.M., A.W.P., and M.T.)

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 pulses coupled with "gateable" multichannel detectors with matched repetition rates and short on-times. Both electronic and optical gating technologies have been shown to significantly improve the Raman spectra of highly florescent *solutions*. However, the performance of such systems with *solid* materials has not been reported in detail. To partially redress this imbalance, this article describes the ps-time-resolved Raman spectroscopy of solid films and powders. Excellent temporal resolution and fluorescence rejection was obtained with homogeneous films, but with powders, multiple scattering has the potential to significantly blur the time resolution. For example, after incidence of a 1-ps pulse on a powdered 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 that predict 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 incompletely captured within the short detector "on" period. The fluorescence would be rejected, but so would the Raman signal (to some extent), giving a poor signal-to-noise ratio. This long-term 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. 1701 - 1707
Meggers Award

Generalized Implementation of Rapid-Scan Fourier Transform Infrared Spectroscopic Imaging

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We describe a novel, generalized data acquisition sequence to allow rapid-scan Fourier transform infrared (FT-IR) spectroscopic imaging using focal plane array (FPA) detectors. This technique derives its applicability from the reproducible performance of modern FT-IR instrumentation and the availability of FPAs with simultaneous, full array acquisition, or snapshot electronics. Instead of sampling the entire interferogram in one mirror sweep over a predetermined retardation, as in traditional continuous-scanning techniques, the modulated light from the interferometer is recorded over several mirror sweeps. The FPA detector is synchronized for data acquisition after a specified delay with respect to the initiation of the mirror motion to provide a highly under-sampled interferogram. By incorporating appropriate delays in subsequent interferometer mirror scans, the entire interferogram is sampled and reconstructed. The signal-to-noise ratios (SNR) of the resulting interferograms are analyzed and are compared with step-scan spectroscopic imaging data.

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

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

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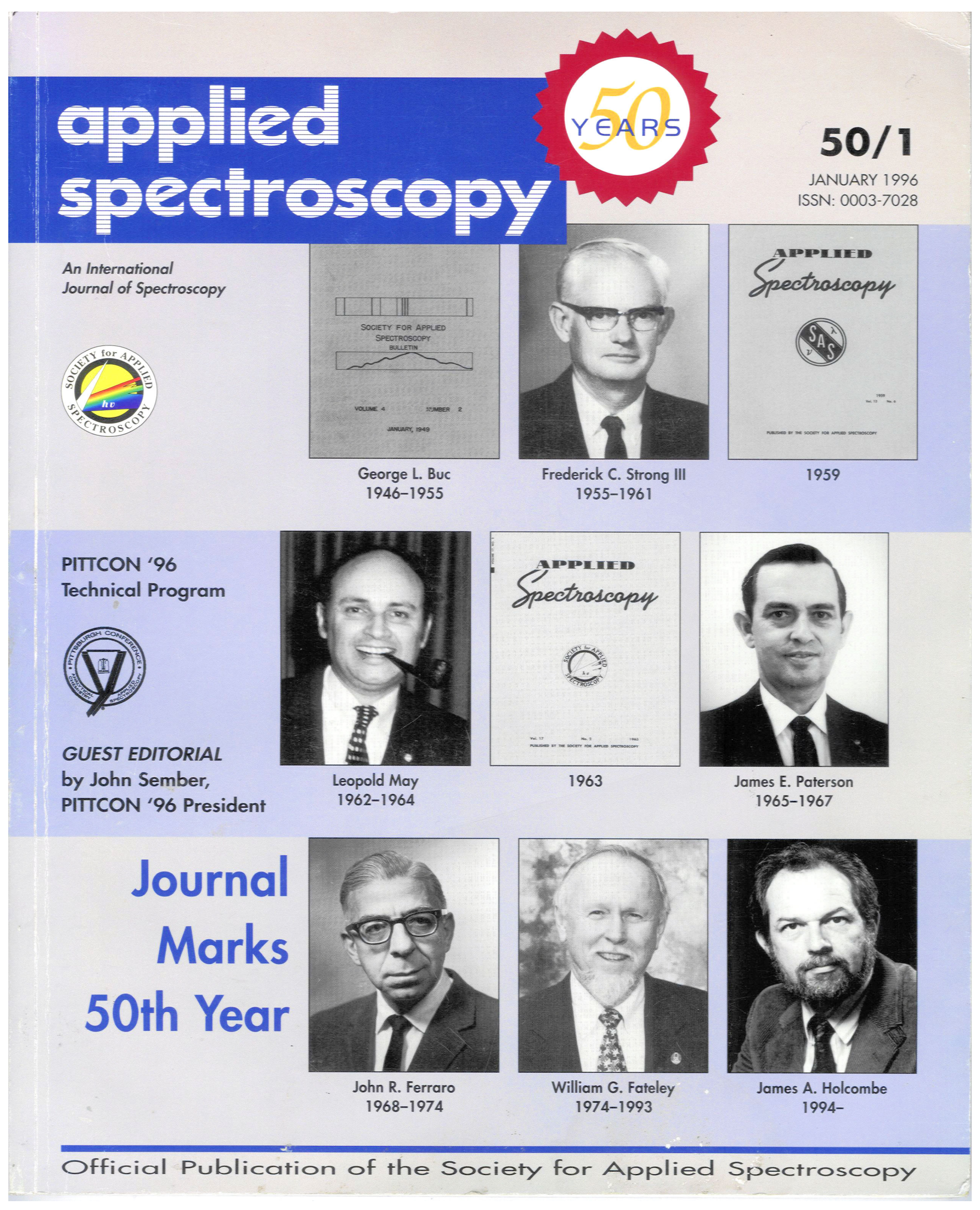
We present the first elementary model predicting how Raman intensities vary for a range of experimental variables for spatially offset Raman spectroscopy (SORS), a recently proposed technique for the effective retrieval of Raman spectra of subsurface layers in diffusely scattering media. The model was able to reproduce the key observations made from the first SORS experiments, namely the dependence of Raman signal intensities on the spatial offset between the illumination and collection points and the relative contributions to the overall spectrum from the top layer and the sub-layer. The application of the SORS concept to a three-layer system is also discussed. The model also clearly indicates that an annular geometry, rather than a point-collection geometry, which was used in the earlier experiments, would yield much improved data.

Volume 59, Number 12, 2005, pp. 1485 - 1492
Meggers Award



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Frederick C. Strong III 1955–1961
1959
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Leopold May 1962–1964
1963
James E. Paterson 1965–1967
Journal Marks 50th Year
John R. Ferraro 1968–1974
William G. Fateley 1974–1993
James A. Holcombe 1994–
Official Publication of the Society for Applied Spectroscopy

In mid-1945, as World War II neared its end, a group of scientists in and around New York City formed a new organizations, 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 seven Editors-in-Chief during the first fifty years. Two of them, John Ferraro and Leopold May, also served terms as President of SAS.