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EBOOK

CHEMISTRY & SPECTROSCOPY

BY AVANTES - EMPOWERING SPECTROSCOPY SOLUTIONS

WELCOME

A crucial part of Avantes’ mission statement refers to providing state-of-the-art, innovating measuring equipment that helps humankind live longer and healthier. By offering our empowering spectroscopy solutions to researchers, chemists, and Original Equipment Manufacturers, we can contribute to that mission and help them achieve their measurement challenges.

With almost 30 years of experience, Avantes is an equipped partner to guide customers to a spectroscopic solution tailored to their application and research needs.

Curious how spectroscopy can help you reveal answers by measuring all kinds of materials in-line at your production facility, in a lab, or the field? Please get in touch with one of our technical experts. We are happy to help!

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INTRODUCTION

SPECTROSCOPY IN CHEMISTRY

Chemical applications for spectroscopy are innumerable and increasing every day. Chemical reactions are dynamic processes that present unique challenges ranging from temperature fluctuations to corrosive and caustic attributes, which require robust analytical techniques and tools. Monitoring chemical reactions in the food/beverage, petroleum, semiconductor, and chemical industry provide a valuable tool for quality control. Non-invasive and in-situ spectroscopy analysis facilitated by Avantes instruments and accessories provide real-time, high-speed measurements of chemical processes.

With the help of spectroscopy, you can measure concentrations, process endpoints, and contamination at concentrations as low parts per billion (ppb). The study of chemical kinetics is used to characterize processes and improve our understanding of how these factors and others change the outcome of a chemical reaction.

In this eBook we dive into different measurement techniques, applications and help you find your ideal measurement setup. Read further to discover all the possibilities spectroscopy has to offer.

1

SECTION 1

MEASUREMENT TECHNIQUES

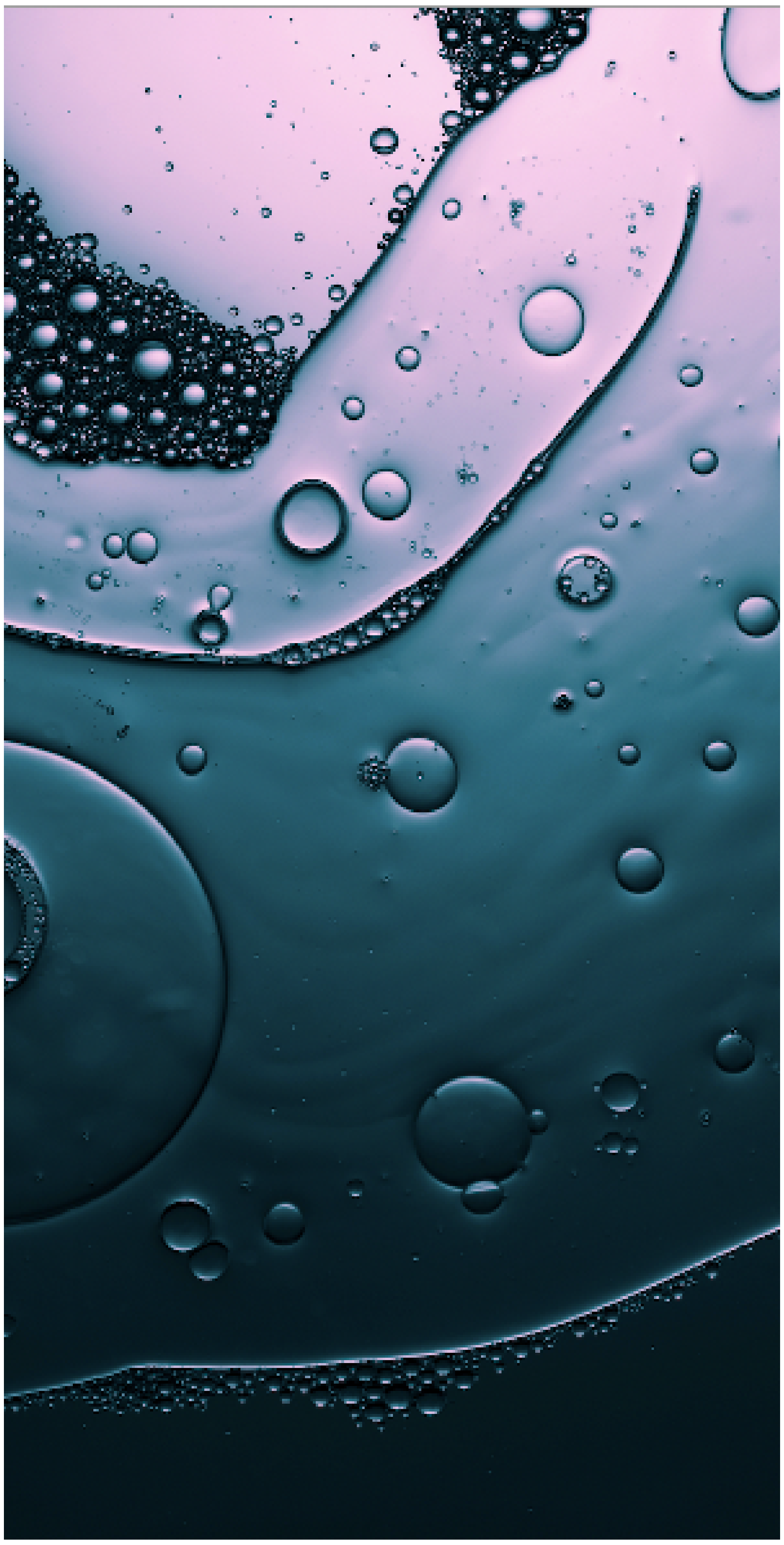
There are an unlimited number of applications in the field of chemical spectroscopy. Chemical reactions are dynamic processes that vary with changing conditions which result from various types of measurement techniques. In this section we will go over a few of them.

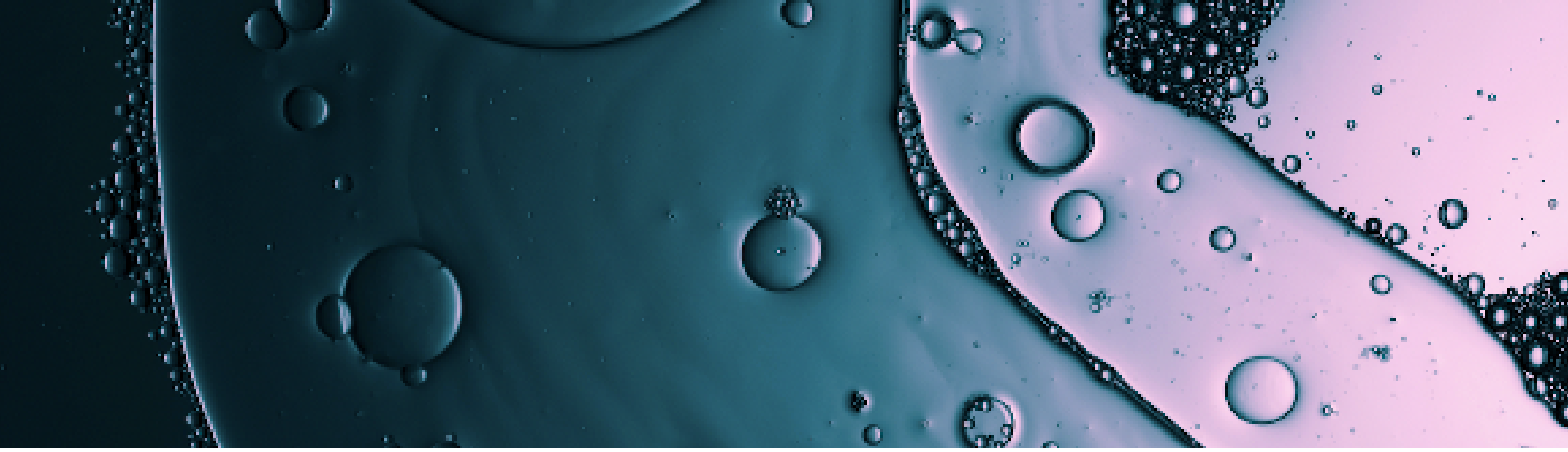
1.1 Beer-Lambert Law

Chemical concentrations can be determined using a variety of techniques derived from Beer-Lambert law analysis. Liquid and gas phase samples can be analyzed over the range from 200-2500 nm and concentrations may be derived using single and multivariate models. Avantes offers a variety of sample interfaces to facilitate laboratory cuvette measurements as well as inline measurements using flow cells and transmission probes. Complex chemical matrices such as volatile organics and carbohydrates may require sophisticated multivariate modeling techniques such as PSA, PLS I & II.

1.2 Raman Spectroscopy

One of the fastest-growing techniques for monitoring chemical reactions is Raman Spectroscopy. A vibrational molecular technique that utilizes an excitation laser, Raman spectroscopy is ideal for material identification, reaction monitoring, remote sensing, and many other applicable measurements. Raman provides a molecular fingerprint for chemical species and allows for the monitoring of changes in molecular bond structures (e.g. state changes and stresses & strains). Avantes high-sensitivity SensLine spectrometers are ideally suited for Raman spectroscopy.





1.3 Fluorescence

Fluorescence spectroscopy is another molecular technique that may be used to investigate the behaviors of chemical compounds. This technique is a type of photoluminescence where light energy elevates an electron in a sample to an excited state. This excited state then has a rapid thermal energy loss to its environment due to its vibration, and then it emits a photon from its lowest-lying singlet excited state. It is a valuable technique in many biological (chlorophyll and carotenoid), biochemical (protein quantification, fluorescence diagnosis of malignancies), and environmental (Contaminant detection) applications.

1.4 Spectroelectrochemistry

Spectroelectrochemistry (SEC), another analytical technique, involves the combination of electrochemistry with spectroscopy as electrical potential is applied to chemical samples while simultaneously being measured spectroscopically. Spectroscopic information about electrogenerated species can be obtained, including electronic absorption, vibrational modes and frequencies, light emission and scattering, magnetic resonance, and circular dichroism. Avantes instruments perform exceptionally well in this application due to the sophisticated electronics controls facilitated by our AS7010 (EVO) electronics and accompanying controlling software.

2

SECTION 2

APPLICATIONS

Chemistry touches so many aspects of our lives that you are guaranteed to find chemistry at the forefront of many advances and developments. And you can trust that Avantes will be there to support you with your applications. Avantes' decades of experience developing custom-designed systems for chemistry applications mean researchers can count on us for reliability and ease of use.

2.1 In-situ UV-vis-NIR Spectroelectrochemistry on electrochromic materials

INTRODUCTION METHODOLOGY

UV–vis–NIR spectroelectrochemistry is a combination of cyclic voltammetry (CV) and absorption spectroscopy in ultraviolet, visible, and near-infrared regions of the electromagnetic spectrum. Electron transfer reactions at electrodes result in changes of the electronic structure of the electroactive species. These changes and their influence on the spectroscopic response of the compounds form the background of any spectroelectrochemical method. Thus, coupling cyclic voltammetry measurement with measurement of absorption spectra can give valuable information on the mechanismof the electrochemical reactions, the types of the formed charged species, and their electronic structure. The in-situ spectroelectrochemical method enables sensitive spectroscopic measurements under electron transfer conditions. Due to the accuracy of the technique, the formation of charged species and the evolution of their concentration in dependence on applied potential can be followed. UV–vis–NIR spectroelectrochemistry is the method of choice to study the redox processes in electrochromic materials. These materials can reversibly change their color as a result of an electrochemical reaction and are an essential component in all kinds of electrochromic devices (ECDs). For the development and production of tailored ECDs, it is important to understand the mechanisms of the electron transfer reactions in such materials and to identify the species which are responsible for the coloration.

Applications of UV–vis–NIR spectroelectrochemistry to study on electrochromic materials include:

- Real-time monitoring of electrochromic changes by redox reaction
- Spectroscopic detection and identifying the species responsible for the coloration
- Study of the optical properties and stability of charged species
- Concentration profile of (colored) species in dependence on stepwise varying potential
- Elucidation of the mechanisms of electrochemical reactions

INSTRUMENTATION

AvaSpec Spectrometers (single or multi-channel):

For most applications, the broadband configuration (200-1100 nm) of the AvaSpec-ULS-2048CL-EVO is used but for broader coverage, additional spectrometers can be added such as the AvaSpec-NIR256-2.-HSC-EVO (allowing for 200-2500 nm measurement) Each spectrometer can be configurated independently but can be synchronized and the spectral data can be merged. The whole spectrum is measured at once in milliseconds.

AvaLight- light sources:

The Avalight-DHc and Avalight-DH-S-BAL are both balanced deuterium and halogen light sources, in which the alpha peak at 656 nm is significantly reduced. An integrated TTL-shutter can be triggered by the spectrometer or potentiostat.

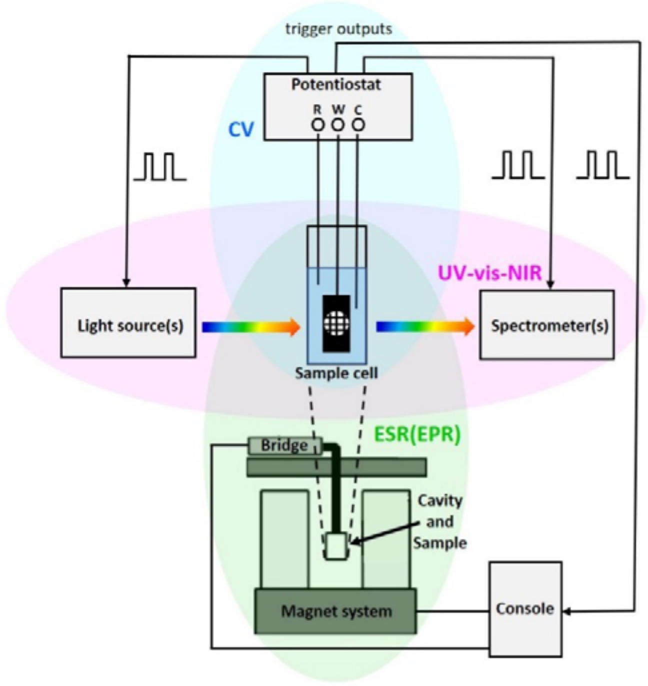


FIGURE 1
Spectroelectrochemical setup

Potentiostat: Any potentiostat that provides TTL trigger outputs can be used for triggering the spectrometer. The Digital Input/Outputs (DIO) offer the possibility to synchronize electrochemical measurements with external devices controlled by TTL signals. To trigger the acquisition of the spectra on the spectrometer and control the shutter of the light source, a dedicated trigger cable is required. This cable is used to connect the EXTERNAL I/O connector located on the back of the spectrometer to an available DIO port on the potentiostat. The acquisition of a spectrum is triggered by sending a TTL pulse from the potentiostat to the spectrometer and light source. Each pulse triggers the acquisition of one spectrum.

Fiber-optic cables (single or multifurcated):

For single instruments, a simple fiber cable can be used but for multi-channel instruments, bifurcated and multifurcated fiber optics may be required. The so-called multifurcated fibers split out from the light sources to the cell and from the cell to the individual detectors. Avantes fiber optics are configured with our unique broadband fiber which facilitates transmission of light from 200-2500 nm.

OPTICALLY TRANSPARANT THIN LAYER ELECTROCHEMICAL CELL

Needed to couple electrochemistry and absorption spectroscopy in transmission mode. Usually, noble metal meshes or substrates coated with indium-tin-oxide or ultrathin layer of noble metal are used as working electrodes. Under thin layer conditions, complete electrolysis of electroactive reactants is rapidly achieved. The interfering reactant absorption is minimized. This is more important in the case of consecutive electron transfer reactions. Cells with optical path lengths of 1.0, 0.5, or <0.2mm are available and suited to techniques with simultaneous spectroscopic characterization of reaction products under finite and semi-infinite diffusion conditions.

CASE STUDY ON VIOLOGEN SYSTEMS

Viologens (1,1’-disubstituted-4,4’-bipyridinium salts) are widely established as organic electrochromic compounds. The three common redox forms of viologens are the usually colorless dication, the highly colored radical cation, and the di-reduced (neutral) form. The radical cation and neutral form are generated by two consecutive reductions. The Spectroelectrochemistry group at the Leibniz Institute for Solid State and Materials Research (Germany) headed by Dr. Evgenia Dmitrieva, together with the CIDETEC Technology Centre (Spain) studied a series of viologen compounds in by in situ UV-vis-NIR spectroelectrochemistry (Fig. 2).[1], [2] The electrochromic properties of the viologen systems can be modulated by varying the molecular structure of the viologens (substituents at the nitrogen atoms) and also by changing their environment (electrolytic media). ECDs based on symmetric compounds (R = R´) with alkyl substituents show violet coloration, while viologens with aryl groups demonstrate green coloration for their first reduced form (radical cation). ECDs based on asymmetric viologens (R ≠ R´) may provide more neutral (greyish) coloration[3].

EDCs containing anhydrous organic solvent (propylene carbonate) and polyvinyl alcohol (PVA) – borax hydrogel as a polyelectrolyte demonstrate a different coloration. UV–vis–NIR spectra measured in PVA-borax gel during the reduction of ethyl viologen are shown in Fig. 3b and c .The analysis of the absorption spectra reveals three distinct patterns corresponding to the radical cation (V•+) and π-dimer $(V^{\bullet +})^2$ formed during the one electron reduction.

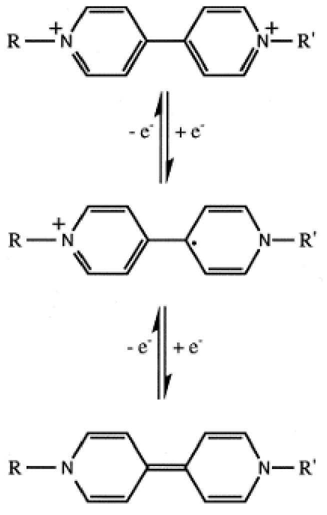


FIGURE 2

Three common viologen redox forms
R, R' = alkyl or aryl group

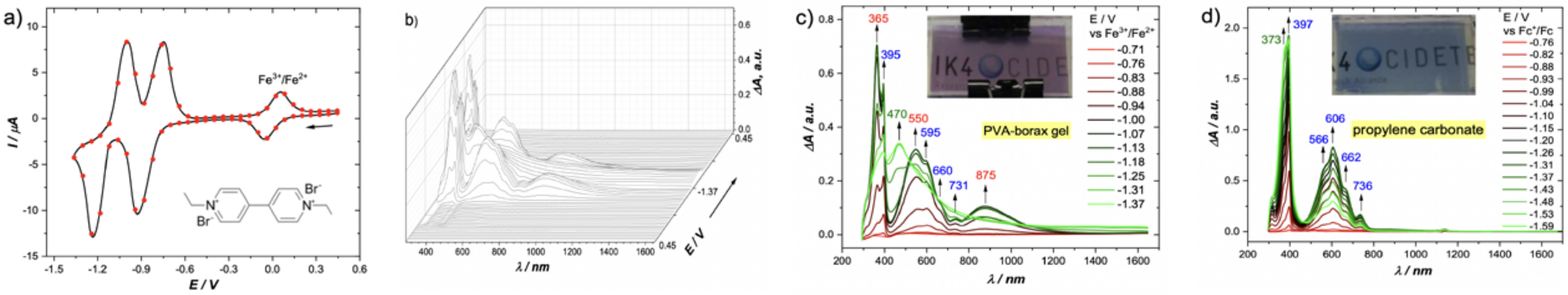
Electrolytic medium	UV–vis–NIR bands (λ_{max}, nm)		
	radical cation ($V^{\bullet +}$)	dimer $(V^{\bullet +})_2$	neutral form
PVA-borax gel	395, **595**, 660, 731	365, **550**, 875	395, 470
propylene carbonate	397, 556, **606**, 662, 736	–	373, 397

TABLE 1

Assignment of the UV–vis–NIR absorption bands observed during reduction of EtV^{2+}. The dominant bands in the visible range are shown

Di-reduced structures are observed during the two-electron reduction (Table 1). The dimers are characterized by the bands which are blue-shifted compared to that of the radical cation and a pronounced charge-transfer band in the near infrared region. During the one-electron reduction ECDs provide a violet coloration in consequence of the absorption at 595 (blue radical cation) and 550 (purple π-dimer) nm (Fig. 3c, inset). Based on the spectroscopic data, it can be concluded that a large amount of the π-dimers are formed in PVA-borax gel and they significantly contribute to the color observation. In contrast to the polyelectrolyte, in polar organic solvents such as propylene carbonate no dimers are formed because ion pair formation precludes dimerization. In this case the device coloration is only caused by the absorption of the radical cation (Fig. 3d, inset). As summary, UV–vis–NIR spectroelectrochemistry on electrochromic compounds provides information about what kind of charged species are formed during the electrochemical treatment as well as their optical properties depending on experimental conditions.

FIG. 3A, B, C & D



Cyclic voltammogram of ethyl viologen EtV^{2+} (Fig 3A) and 3D plot of the UV-vis-NIR spectra (Fig 3B) measured in PVA-borax gel during the reduction of EtV^{2+}. Potentials at which the spectra were measured are marked by red points. 2D plot of the UV-vis-NIR spectra recorded in PVA-borax gel (Fig 3C) and propylene carbonate containing 0.2 M TBABF^4 (Fig 3D). The spectrum of the solution containing 3.5 mM EtV^{2+} recorded at initial potential was taken as a reference spectrum.

COMBINATION ESR SPECTROSCOPY

The electron spin (paramagnetic) resonance (ESR/EPR) spectroscopy is the method of choice for the detection and characterization of structures containing unpaired electrons (e.g. organic radicals, transition metal ions). A primary step of the electron transfer in a neutral organic molecule leads to the formation of a radical ion, which can be unambitiously confirmed by ESR spectroscopy. A second electron transfer usually results in diamagnetic structures. UV–vis–NIR spectroscopy delivers information about the optical properties of both paramagnetic and diamagnetic species. Polyelectrolyte-based ECDs containing p-cyanophenyl viologen and PVA-borax gel provide two different well-defined colored states (Fig. 4a). The application of the less negative potential leads to the observation of green coloration, while the more negative applied potential generates a red one. By using the triple method (combination of cyclic voltammetry, electron spin resonance, and electronic absorption spectroscopy) it is possible to identify the species responsible for each coloration. The dependence of the ESR signal and charge-transfer band intensities on applied potential demonstrates the evolution of the concentration of the radical cation and the dimer (Fig. 4b). The dominant species can be determined at a stepwise varying potential. As result, a complete mechanism of viologen reduction can be elucidated.

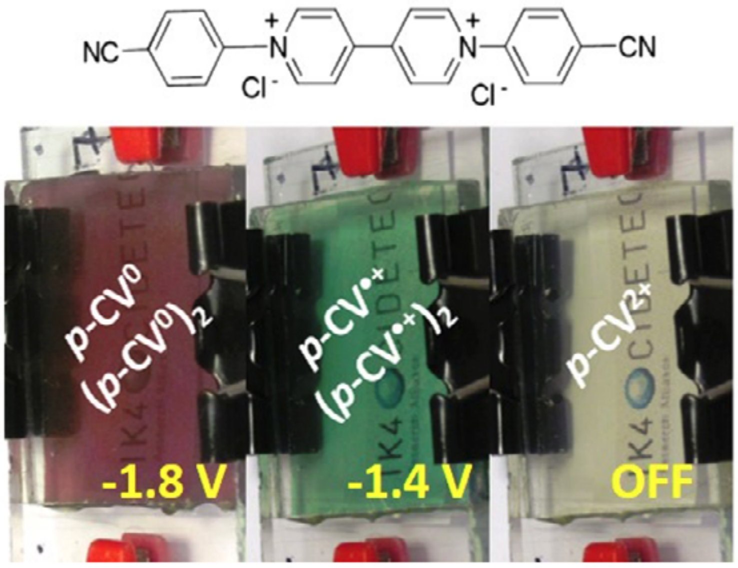


FIGURE 4A
A: Photographs of the device based on p-cyanophenyl viologen p-CNV^{2+} and PVA-borax gel at different applied voltage.
The species responsible for the device coloration are indicated.

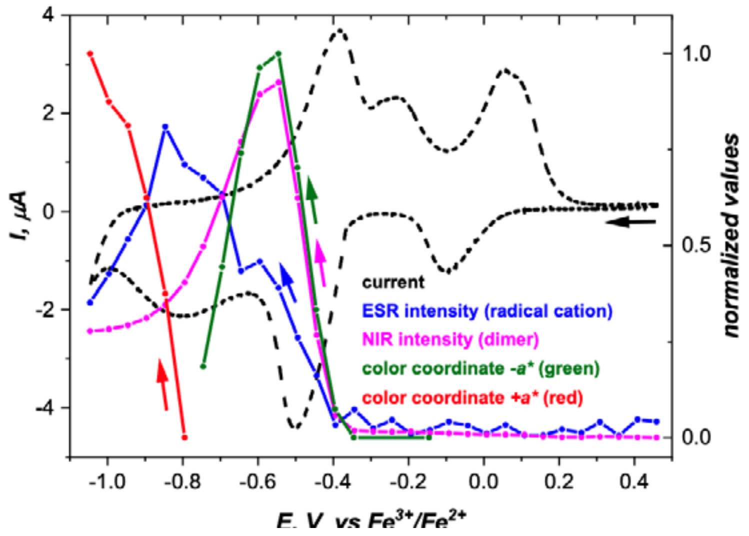


FIGURE 4B
B: Potential profiles of the ESR signal and NIR band intensities as well as color coordinates.

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The reduction mechanism of p-cyanophenylviologen in PVA-borax gel polyelectrolyte-based bicolor electrochromic devices. Electrochim. Acta 292 (2018) 81-87.

2. E. Dmitrieva, M. Rosenkranz, Y. Alesanco, A. Viñuales.
Spectroelectrochemical study of alkyl-aryl asymmetric viologens in poly(vinyl alcohol) (PVA) – borax electrolyte. Electrochim. Acta 323 (2019) 1347992.

3. Y. Alesanco, A. Vinuales, German Cabanero, Javier Rodriguez, and Ramon Tena-Zaera.
Colorless to Neutral Color Electrochromic Devices Based on Asymmetric Viologens. ACS Appl. Mater. Interfaces 8 (2016) 29619–29627

2.2 Improved Plutonium Processing at SRS National Lab

Replacing an aging colorimeter process monitoring system with a cutting-edge spectroscopy system featuring Avantes spectrometers offers promising benefits for the HB Line Chemical Processing Facility at the Savannah River Site (SRS), part of the surplus plutonium disposition mission. The new system, developed in partnership with Department of Energy Office of Environmental Management, employs commercially available spectrometers and is proving to be easier to troubleshoot, repair, and calibrate than the old system. It also improves efficiency and safety for employees, staff, and the environment.

THE SAVANNAH RIVER COMPLEX

Commissioned in 1951, in the early years of the Cold War, the Savannah River site was initially built to produce nuclear material, primarily Plutonium-239, for use in weapons programs. The Savannah River Complex consists of several reactors as well as support facilities including chemical separation plants and waste management facilities. The HB Line facility is the hardened nuclear chemical separations plant for recovering nuclear material and producing material to fuel the nation's deep space exploration program.

HB LINE PROCESS MONITORING

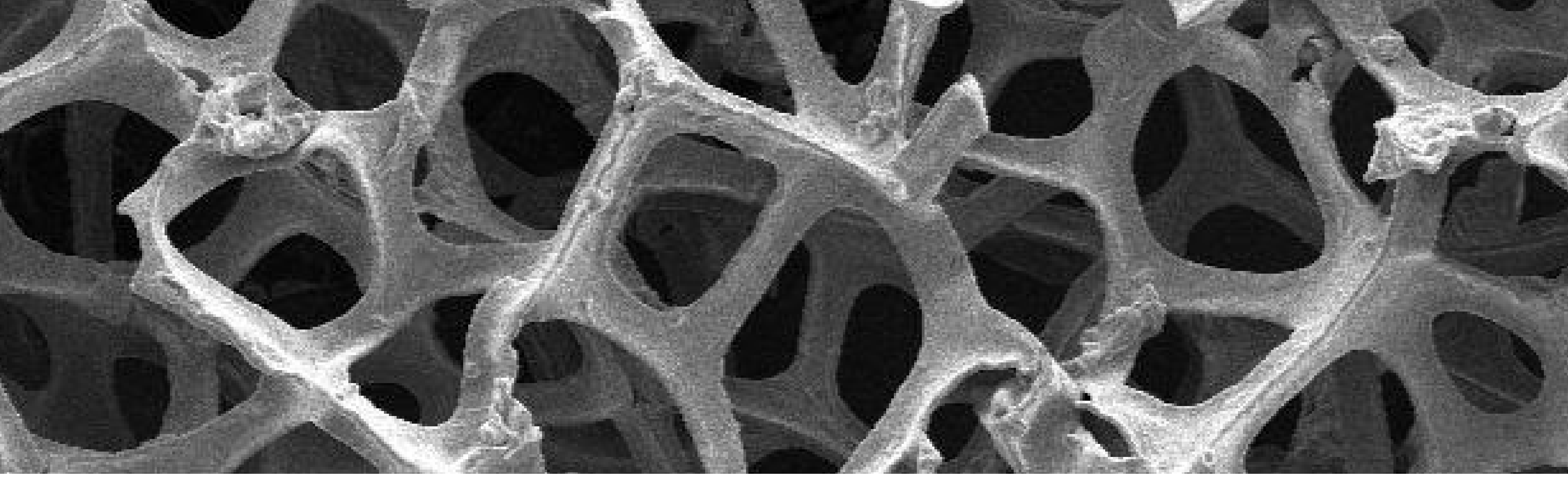
The HB Line historically employed colorimeters to detect plutonium concentrations in solutions. The darker the color of solutions, generally the higher concentration of plutonium. These instruments required downtime to troubleshoot and repair, and required annual off-site calibration. The colorimeter instruments also lacked accuracy requiring the team to keep concentrations low to be certain they stayed within safety margins.

NEXT-GENERATION SPECTROPHOTOMETER

The new process control system is called the Next Generation Spectrophotometer (NGS). Housed in a rack mount cabinet in the HB Line operations control room, the NGS system is comprised of several paired dual-channel spectrometers, roughly 10 pairs. Because the spectrophotometer system can detect a broader range of colors, the measurements are more accurate. The rack mount design is also easier to maintain and scalable, allowing expansion of the system without the need for hardware or software modification. Employees can calibrate the system within minutes without dismantling the system which reduces downtime, and the user-friendly interface alerts operators of alarm conditions. Because of the increased accuracy of measurements, plutonium concentrations can average closer to the limits without fear of exceeding.

LEADING EDGE SPECTROMETERS

The dual-channel spectrometer pairs of the NGS at the Savannah River HB Line are based on the Avantes AvaSpec-ULS4096CL-EVO which is part of the Starline product category. This instrument offers exceptional UV response covering 200-1100nm and is sensitive to 160,000 counts/μW per ms integration time. The configuration used also features a custom version of Avantes BSD-DA (direct attached beamsplitter/combiner) which facilitates periodic inline referencing to correct for light source drift. The improvements to accuracy and maintenance time are dramatic for this section of the Savannah River site and there is potential for this system to be implemented in other areas of the Department of Energy.



2.3

Photoluminescent Response in Graphene Foam

Material science and engineering entail the design and discovery of new materials. This discipline incorporates the work of chemistry, physics, engineering along with ceramics, metallurgy, nanotechnology, biomaterials, and others. The understanding of processing methods, physical and chemical structure, and the properties or behavior of materials is the heart of the materials paradigm. There are numerous historical examples of scientific progress limited by available materials so that breakthroughs in material science are often followed by advances in other areas of research. Material science can arguably be considered the oldest example of engineering and applied science. In fact, material sciences are so important that we often separate historic periods by the material discoveries of the age, such as the Stone Age, Bronze Age, Iron Age, and what today could be considered the 'Silicon Age'. Material science is responsible for the discoveries of rubbers, plastics, semiconductors, and biomaterials, to name just a few.

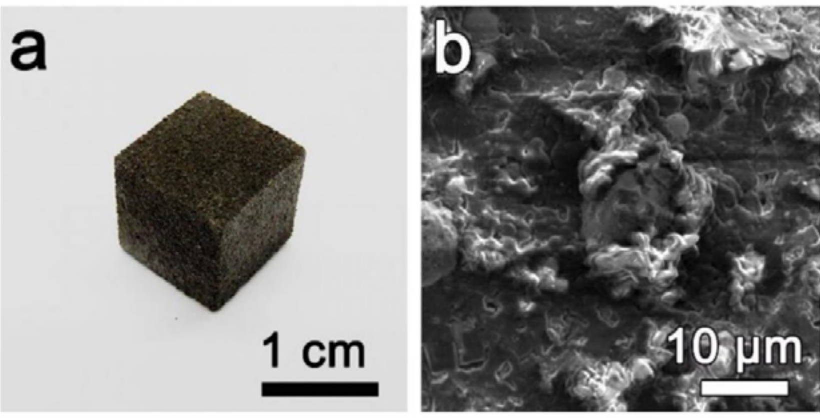
Spectroscopy has several applications in material science, from material identification to process and quality controls. Raman spectroscopy can provide insight into crystalline alignment, laser-induced breakdown spectroscopy is used to identify the atomic composition, and emission monitoring spectroscopy analyzes plasma composition during chemical deposition processes. Avantes spectrometers are there, trusted around the world to deliver accurate spectral measurements for material scientists.

GRAPHENE BREAKTHROUGHS

Graphene is a semi-metallic material that consists of a single layer of carbon molecules in a hexagonal grid arrangement and is the base structural element of other carbon-based materials such as graphite, diamonds, and carbon nanotubes.

This material has several unusual and unique properties. It is so thin that it is considered two-dimensional, yet it is the strongest material ever discovered. Graphene is also a zero-bandgap semiconductor with surprising opacity for an atomic monolayer material. Because it is a zero-bandgap conductor, the light-emitting capacity is limited and pristine graphene is not considered a likely candidate for light-emitting devices.

Derivatives of graphene, on the other hand, such as oxidized graphene, graphene quantum dots, and carbon nanotubes have been observed emitting broadband white light emissions when subjected to focused infrared irradiation in a vacuum.



GRAPHENE BREAKTHROUGHS

Graphene foam is created using chemical vapor deposition which creates self-assembled sheets of oxidized graphene deposited on a three-dimensional mesh of metal filaments, after which the metal is removed. The resulting graphene foam is resilient, returning to its original shape after compression and able to support 3,000 times its weight. This mechanical strength, flexibility, and elasticity make this lightweight, high-conductive material an excellent candidate for several engineering applications.

The conductivity of graphene foam is also being explored for the development of flexible batteries with greater energy density than standard commercially available batteries. Another ely application is in chemical sensing with the ability to detect 20 parts-per-million of Nitrogen Dioxide.

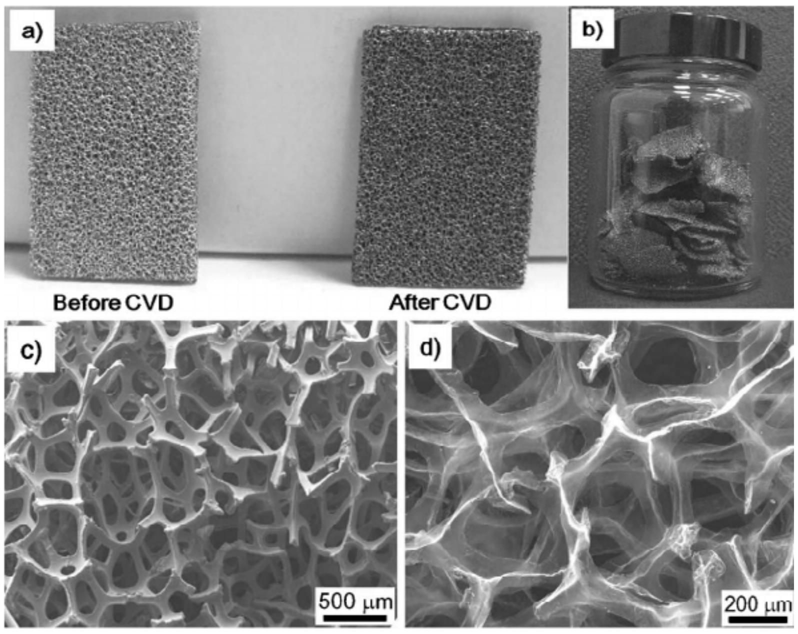


FIGURE 1
Zhao, Guixia, et al. 'Synthesis of graphene-based nanomaterials and their applications energy-related and environmental-related areas.' Rsc Advances 2.25 (2012): 9286-9303.

LASER-INDUCED WHITE LIGHT EMISSION

Researchers at the Polish Academy of Sciences from the departments of Low Temperature and Structure Research and Spectroscopy of Excited States investigated the light emission capacity of graphene foams. Following related research into light emission from irradiated quantum dots and induced incandescence of carbon nanotubes, these scientists were able to achieve white light emission from graphene foam irradiated with a sustained, focused, continuous-wave infrared laser diode.

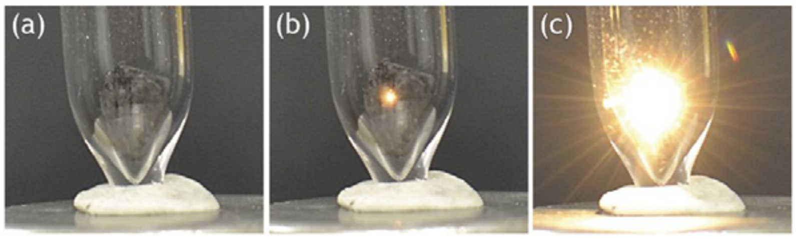


FIGURE 2
(a) the graphene foam in a vacuum cuvette; (b) the photo of the graphene foam emission demonstrating lighting only from the spot at surface of graphene foam; (c) The photo of laser-induced intense white-light emission of the graphene foam. -Strek, Wieslaw

These Laser-Induced White-light Emission (LIWE) experiments were able to achieve white-light emissions with sustained excitation using a 975 nm continuous wave laser diode in a vacuum chamber. This light emission from the graphene foam placed in an integrating sphere under vacuum was limited to the dimensions of the focal point of the excitation laser but demonstrated stable light characteristics that increased in intensity with a corresponding increase in laser power density.

SPECTROMETER UTILITY

These researchers employed Avantes instrumentation during experimentation to measure the photoluminescence response of the graphene foam. While an older instrument was used in the original research, the AvaSpec-ULS2048CL-EVO would be an ideal instrument for this application.

Additionally, spectroscopy can be utilized in the chemical deposition process for graphene foam fabrication for endpoint detection and process control, and morphology or crystallinity can be detected using Raman spectroscopy methods. AvaRaman-532HERO-EVO turnkey Raman system, as well as the AvaSpec-HERO and AvaSpec-ULS2048X64TEC-EVO spectrometers, have been used successfully for graphene characterization via Raman.

In the study of materials, one of the key principles is that the structure at an atomic level determines the behavior of the material on a macro scale. Spectroscopy gives researchers in this field the tools they need to develop the cutting-edge materials of the future.

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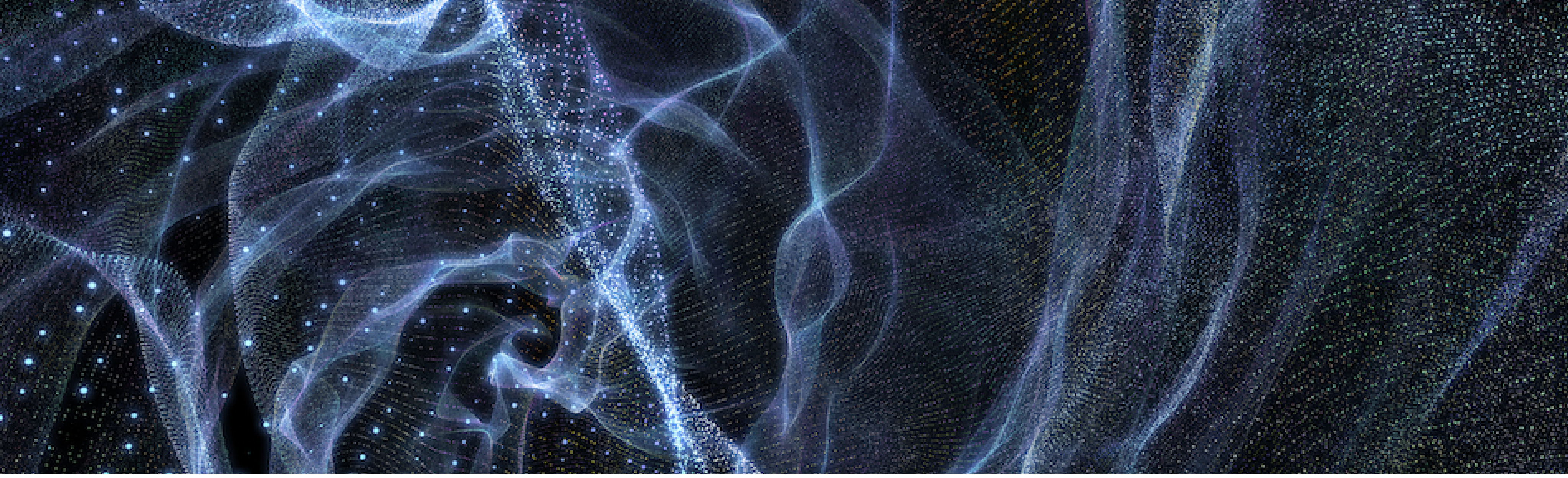


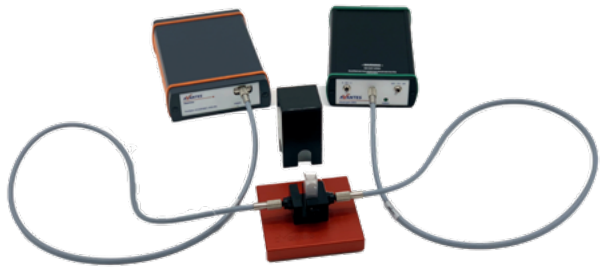
2.4

VIS/NIR Spectroelectrochemical Response

This feature was provided by Pine Instruments as an example of a spectroelectrochemistry application[1] that measures electrochemical response over a range of applied electrical potential and correlated against energy absorption by wavelength. Researchers Greenlee, et al. were measuring the electrochemical response of PMDI's that were functionalized with 4-(dimethylamino) pyridinium (DMAP+) groups. The functionalization resulted in a shift in the reduction potential of the PMDI. The electrochemical technique cyclic voltammetry was used to determine the new reduction potentials of the functionalized PMDIs.

EXPERIMENT PARAMETERS

Wavelength Range	400nm to ~1000nm
Electrical Potential Range	-48.9 mV to -449 mV
Time	300 conds



SYSTEM DESCRIPTION

In such an experiment there are three major components, the spectroscopy equipment (spectrometer and light source), the potentiostat, and the spectroelectrochemical cell. Researchers typically use an optically transparent electrode, made out ITO or a platinum mesh, as the working electrode; Pine Research Instrumentation developed a honeycomb electrode designed to optimize both to rapidly electrolyze the molecule and increase its absorbance compared to the more traditional ITO and platinum mesh electrodes.

A potentiostat is used to apply a potential to the electrode to induce an electron transfer. Then the researcher collects UV/vis spectra of the oxidized or reduced species using their light source and spectrometer.

INSTRUMENTATION

- Due to its exceptional response speed, the AvaSpec-2048CL-EVO is particularly useful in time-critical situations. In this configuration, a UA grating was implemented to give the spectrometer a broadband range of 200 nm to 1100 nm. The detector in has a native UV response, and the configuration includes a linear variable and a 50-micron slit.

- The AvaLight-DHc light source has controllable deuterium and halogen light sources. Deuterium emits light between 200 and 550 nm, halogen emits up to 2500 nm, providing adequate light between 200 and 2500 nm for absorbance chemistry applications. Due to its low output energy, it's recommended for small pathlength measurements or direct attachment to a cuvette holder, such as the CUV-DA. The integrated TTL-shutter makes saving a dark measurement easy and allows for faster measurements as the bulb doesn't have to be turned off and on with the warm-up period.

- (2) 600-micron diameter fibers, 2 meters long each
- Cuvette holder
- A Pine Research WaveNow potentiostat -benchtop, research-grade electrochemical workstation

DATA ON ABSORPTION AND ELECTROCHEMICAL RESPONSE

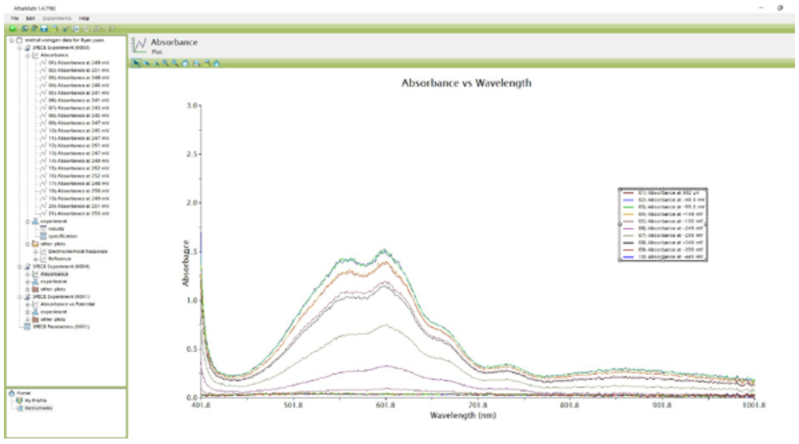


FIGURE 1:
Absorption Response vs. Wavelenght

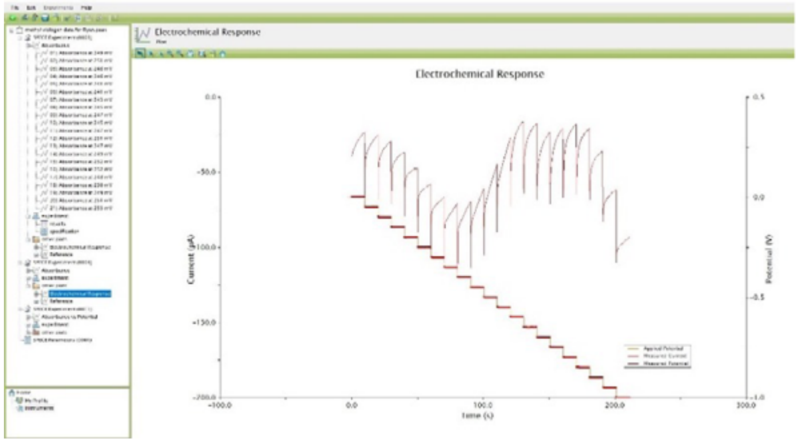


FIGURE 2:
Electrochemical Response

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Andrew J. Greenlee, Charles K. Ofosu, Qifan Xiao, Mohammed M. Modan, Daron E. Janzen, and Dennis D. Cao. ACS Omega 2018 3 (1), 240-245 DOI: 10.1021/acsomega.7b01887

2.5

Absorbance of Food Colorant (ATR Probe)

Absorbance spectroscopy can bring entirely new perspectives on samples through a wide range of industries. This includes industrial lines, where continuous monitoring of water, fluids, and chemicals is necessary to ensure consistent quality and specifications. Many inline control systems use UV/VIS absorbance systems to control quality and ensure process parameters are maintained. A common tool for these types of systems is flow cells and transflectance probes (aka dip probes), where an optical path length is used to measure light absorbed and transmitted by a liquid sample. A common challenge with this type of optical sampling is that most of these systems cannot measure highly absorptive samples. Samples with absorbance unit values above 4 often preclude the use of traditional UV/VIS absorbance measurements. A means of overcoming this limitation is through the use of attenuated total reflectance (ATR).

ATR uses the property of total internal reflection through a crystal resulting in an evanescent wave. A beam of visible or near-infrared light is passed through the ATR crystal in such a way that it reflects several times off the internal surface in contact with the sample. This reflection forms the evanescent wave which extends into the sample medium which may be a liquid, slurry, or solid. The penetration depth into the sample is typically between 0.5 and 2 microns, with the exact penetration value being a function of the wavelength of light, the angle of incidence, and the indices of refraction for the ATR crystal and the medium being measured. As the beam exits the crystal, it is collected by a spectrometer.

ATR is an ideal technique for measuring high concentration samples such as inks, dyes, or dark solid samples such as coal, sludge, etc.

Avantes USA offers an **attenuated total reflectance (ATR) probe** option, which easily couples with our line of AvaSpec spectrometers to facilitate measurements of high absorbance (optical density samples). The AvaPRB-ATR-Z attenuated total reflectance probe is primarily suited to liquid measurements. The probe's robust design is suited for flange mounting inside reaction vessels. In this Spectra of the Month, Avantes USA used the AvaPRB-ATR-Z to demonstrate this powerfultechnique.

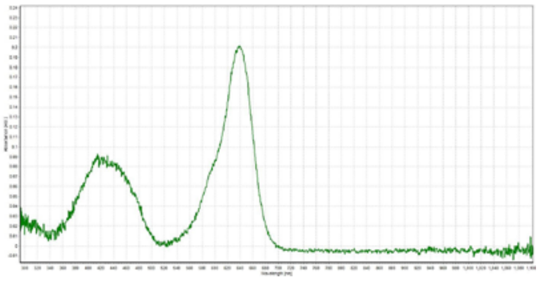
INSTRUMENTATION

For this experiment, we used an **AvaSpec-ULS2048CL-EVO** spectrometer, coupled with an **AvaLight-DHc** light source and the **AvaPRB-ATR-Z probe**. The AvaSpec-ULS2048CL-EVO offers the latest technology, including a CMOS detector, making it a spectrometer platform that will last for many years. In combination with the latest AS-7010 electronics, it is a versatile device including USB3 communication, and a Gigabit Ethernet port for long distance communication. Besides the high-speed communication options, the EVO series spectrometers also offer a fast microprocessor and 50 times more memory capacity, which can facilitate saving up to 35,000 spectra onboard. Furthermore, the AvaSpec-2048CL-EVO is available with a wide range of slit sizes, gratings, and fiber-optic entrance connectors. One popular feature of this instrument is the optional replaceable slit, which allows end-users to easily replace the slit such that it can influence resolution or sensitivity. In this experiment, we used the AvaLight-DHc (described in 2.4), which provides an excellent, broad-spectrum by combining deuterium and halogen into a source.

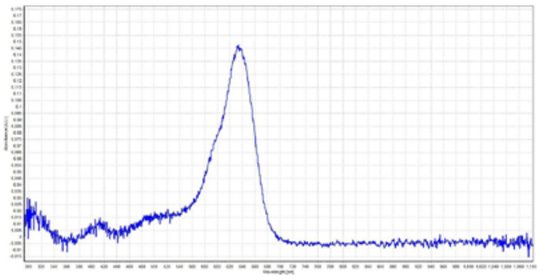
DESCRIPTION OF METHODOLOGY

For this experiment, we utilized the absorbance module in AvaSoft. The absorbance module uses a reference and dark spectrum to measure what wavelengths are being absorbed by the sample. For ATR sampling, either air or a reference solvent (water, ethanol, etc.) can be used for a reference. After the reference and dark spectrums are collected, the ATR probe is submerged in our food coloring samples. We recorded the absorbance spectra of green, blue, red, and yellow food coloring. Typically measurements of food colorants, inks, or dyes require significant dilution down to 10% or lower solutions. For this experiment, the food colorants are measured directly out of the bottle with no dilution.

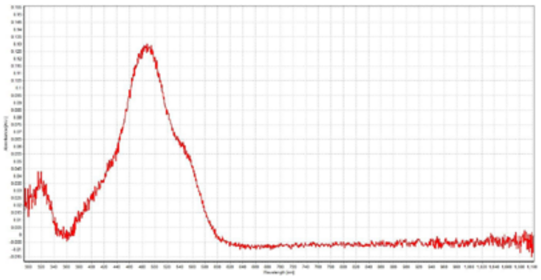
TEST DATA AND RESULTS



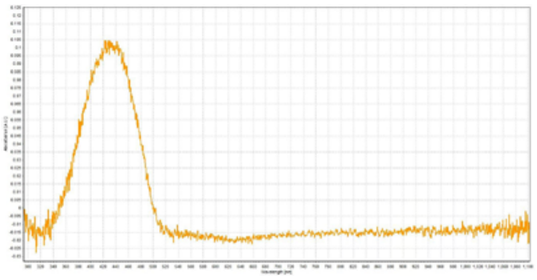
Absorbance spectra for green food coloring



Absorbance spectra for blue food coloring



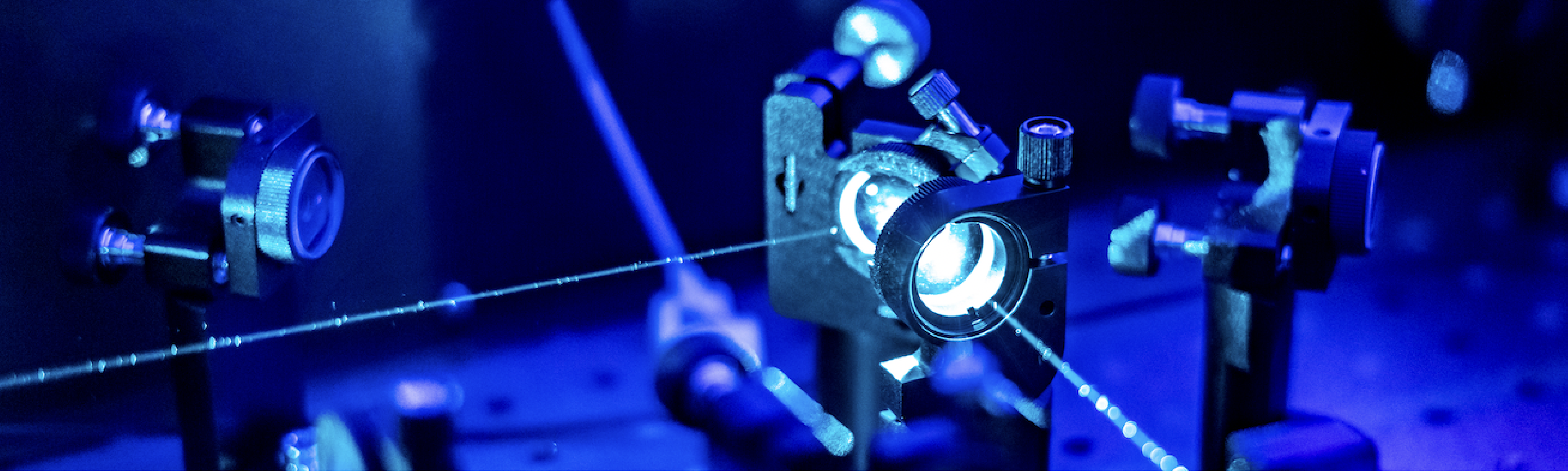
Absorbance spectra for red food coloring



Absorbance spectra for yellow food coloring

ANALYSIS & CONCLUSION

The undiluted food coloring provided an excellent example to prove the effectiveness of an ATR probe in measuring the absorbance values of dense and highly absorbent samples. Had these samples been measured with a dip probe, cuvette, or flow cell, the spectrometer system would have registered noise with absolutely no discernible spectra. Due to the power of the ATR technique, these samples can be measured easily and accurately. These results demonstrate how an ATR probe can be used to consistently measure the color spectrum of inks dyes and other colorants in real time. A near-infrared configuration of the same probe can be used for applications in the 1000-2500 nm range.



2.6 Introduction to Transient Absorption Spectroscopy

When a molecule absorbs a photon, it imparts energy to the molecule, causing it to temporarily excite from the ground state to a higher electronic or vibrational energy level. Due to conservation of energy, absorption can only take place if the photon energy is precisely equal to the difference between the ground and excited states; only then can the light be absorbed. Additionally, since there is a direct correlation between the number of molecules and the number of photons absorbed, it is relatively straightforward to determine the molecular density. As a result, absorption is one of the most commonly used spectroscopic techniques, particularly for concentration measurements.

Most of the excited states induced by absorption are incredibly short-lived. The spontaneous lifetime of most transient excited states is typically on the order of femtoseconds or picoseconds, with the notable exception of meta-stable excited states. Based on this fact, George Porter and Ronald Norrish, while at the University of Cambridge, realized that they could use flash lamps to study these intermolecular energy transitions through a method they called flash photolysis in 1950[1]. Even though the foundation was set in the 1950s, it wasn't until the development of the ultrafast mode-locked laser that scientists could fully take advantage of Porter and Norrish's contributions. Today, ultrafast lasers have completely replaced flash lamps as the preferred excitation source for these types of experiments, and the technique is more commonly referred to as transient absorption spectroscopy (TAS).

FUNDAMENTALS OF ABSORPTION SPECTROSCOPY

Traditionally, absorption spectroscopy has been discussed in terms of the Beer-Lambert Law, which relates the transmitted intensity to the absorption coefficient (α) and the pathlength (z), which can be expressed as follows:

$$I(z) = I(0)e^{-\alpha(\lambda)z}$$

Equation 1

While equation 1 is not the most commonly used expression of Beer's law, it is the most useful for gaining an intuitive understanding of the underlying physics. In this form, we can clearly see that the absorption coefficient is wavelength dependent, therefore resulting in an absorption spectrum. By diving deeper into the absorption coefficient for a given transition, we can show the following relationship:

$$I(\lambda) \propto \cos^2\left(d\,\frac{2\pi}{\lambda}\,n(\lambda)\right)$$

Equation 2

Here we see that the absorption coefficient depends on the transition cross-section () which represents the probability of an incoming photon exciting the sample to an excited electronic or vibrational state and the population difference (N) between the ground state (N1) and the excited state (N2)[2]. Additionally, we can see that the transition cross-section is inversely proportional to the spontaneous lifetime (tsp) of the excited state.

Now we can see that unlike the more simplified version of Beer's law taught in introductory chemistry, the absorption spectrum of a given analyte is not truly based on the molecular concentration, but rather on population difference. Furthermore, since the population difference is itself a time-dependent function based on the spontaneous lifetime, the absorption coefficient also has a temporal dependency associated with it. All of that being said, the population difference can be ignored most of the time because the spontaneous lifetime is so fast, and the light intensity is so weak, that it never significantly depletes the ground state population.

MEASURING TRANSITION LIFETIMES

While there are many different ways to use ultrafast lasers to perform TAS, on the most fundamental level they are all variations on a single technique, known as pump-probe. The procedure requires two laser beams to excite the analyte and measure absorbance simultaneously.

First, the high-intensity pump laser excites a significant percentage of the molecules in the sample to a higher energy level, altering the population difference and reducing the absorption coefficient of the transition. Next, a low-intensity probe laser is passed through the sample to measure the absorption. Based on the difference between the probe laser absorption with and without the pump laser, you can then determine the change in absorption. This process is then systematically repeated for different delay times between the pump and probe pulses to measuring the change in transmitted probe pulse energy, as shown in Figure 1.

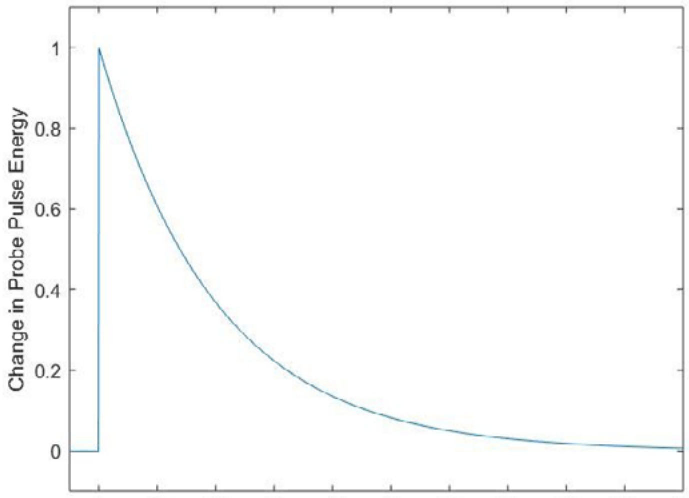


FIGURE 1:
Simulated pump-probe TAS kinetic decay data

From this data, we can build a picture of the kinetics of the energy level transitions and determine spontaneous lifetime and other transient effects.

As referred earlier, we aren't interested in only measuring one transition, but instead, we want to see the effects on the entire spectrum. To accomplish this goal with a monochromatic probe would be impractical, but utilizing a nonlinear optics process known as supercontinuum generation overcomes this issue. An explanation of how supercontinuum light is generated is far beyond the scope of this application note, but it should be understood that this process allows an ultra-short pulse laser to be converted into a white-light source while still maintaining most of the laser properties.

As a result, one can measure the entire spectra with a single probe pulse. Fig. 2 shows a simplified schematic representation of a TAS set-up; a chopper and a lock-in amplifier are added in the system to improve the signal-to-noise ratio. Fig. 3 shows a simulated transient absorption spectrum showing the subtle differences in absorption resulting from the population difference induced by the absorption of the pump pulse.

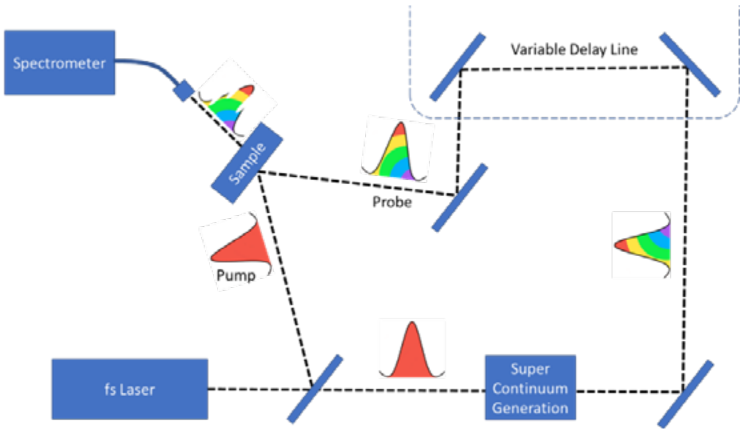


FIGURE 2:
Schematic representation of a typical pump-probe TAS set-up

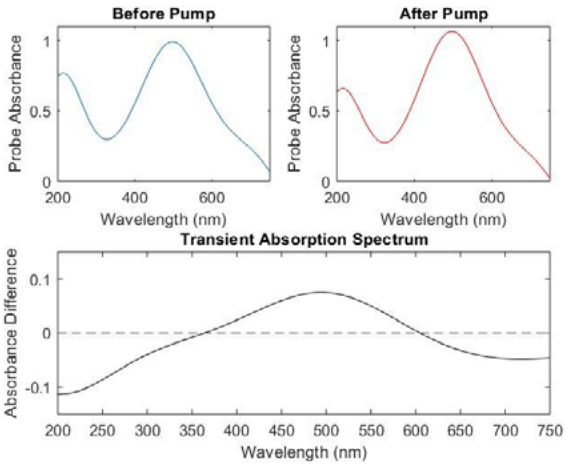
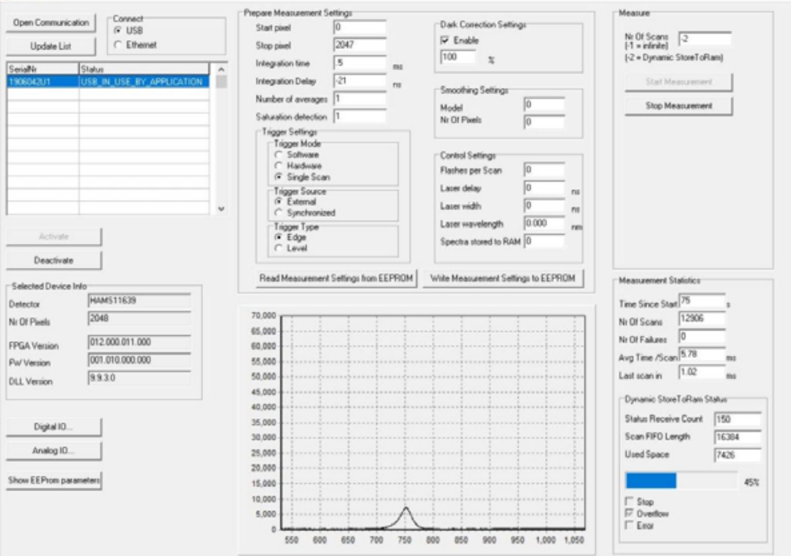


FIGURE 3:
Simulated transient absorption spectrum

MEASURING TRANSITION LIFETIMES

The spectrometer parameters of a typical TAS measurement are very similar to those required for traditional absorption spectroscopy with the exception of speed and dynamic range. First, it should be noted that the speed of data acquisition is in no way correlated to the laser's pulse width or pulse repletion rate. Each spectral integration will contain a large number of individual laser pulses. Instead, the speed requirements are solely dependent on the number of data points that are required to capture the transient kinetics, and how well it can be triggered with the delay line. Additionally, the dynamic range of the spectrometer is so crucial because transient absorption is measured as difference spectra, and the differences can be extremely subtle. As a result, CMOS detectors are always preferable due to their faster readout speeds and larger dynamic ranges than CCD detectors.

Even though the minimum integration time of most CMOS cameras is on the order of 10 microseconds, the major bottleneck is often the spectrometers readout electronics that must transfer the data from the detector to the computer. Avantes' new dynamic store to RAM capabilities represent a significant leap forward in high-speed spectral readout. Utilizing the dynamic store to RAM feature allows the user to save scans to the RAM buffer onboard the instrument and simultaneously offload the spectra to the computer. Using the dynamic store-to-RAM function, the AvaSpec-ULS2048CL-EVO is now capable of continually acquiring spectra at a rate of 2 kHz. Figure 4 shows an example of the new graphical user interface (GUI) when using dynamic store to RAM.



Connect
● USB
○ Ethernet

SerialNr	Status
1906042U1	USB_IN_USE_BY_APPLICATION

Selected Device Info
Detector: HAMS11639
Nr Of Pixels: 2048
FPGA Version: 012.000.011.000
FW Version: 001.010.000.000
DLL Version: 9.9.3.0

Prepare Measurement Settings
Start pixel: 0
Stop pixel: 2047
Integration time: .5 ms
Integration Delay: -21 ns
Number of averages: 1
Saturation detection: 1

Trigger Settings
Trigger Mode
○ Software
○ Hardware
● Single Scan
Trigger Source
● External
○ Synchronized
Trigger Type
● Edge
○ Level

Dark Correction Settings
☑ Enable
100 %

Smoothing Settings
Model: 0
Nr Of Pixels: 0

Control Settings
Flashes per Scan: 0
Laser delay: 0 ns
Laser width: 0 ns
Laser wavelength: 0.000 nm
Spectra stored to RAM: 0

Measure
Nr Of Scans (-1 = infinite) (-2 = Dynamic StoreToRam): -2

Measurement Statistics
Time Since Start: 75 s
Nr Of Scans: 12906
Nr Of Failures: 0
Avg Time /Scan: 5.78 ms
Last scan in: 1.02 ms

Dynamic StoreToRam Status
Status Receive Count: 150
Scan FIFO Length: 16384
Used Space: 7426
45%
☐ Stop
☑ Overflow
☐ Error

FIGURE 4:
Graphical output of Dynamic Store to RAM

APPLICATION EXAMPLE: N-H FISSION IN AQUEOUS ADENINE

The scientific community has widely used Avantes spectrometers for measuring TAS. An excellent example, which visually shows the functionality of TAS data, was published by a group at the University of Bristol while studying N-H bond fission in aqueous adenine[3]. The results shown in Figure 5 below were obtained using an Avantes, AvaSpec-FAST spectrometer (now replaced by the AvaSpec-ULS2048CL-EVO), which used 750 pixels to measure a spectral range from 200 nm to 620nm. The sample was excited with a 266 nm pump laser and a supercontinuum probe laser, with a variable pulse delay from -500fs to 3ps. From this data, it is easy to see the time-dependent nature of the changing absorption coefficient after the pump pulse. Based on the curve fit shown in Figure 5b, the research team was able to determine that the spontaneous lifetime (or 'time-constant' as they referred to it) was 470 +/- 18 fs[3].

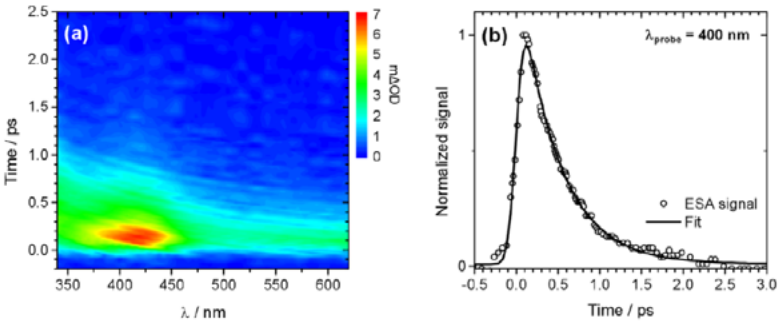


FIGURE 5:
(a) Waterfall plot of TAS spectra of Ade[-H] in D2O excited with a 266 nm pump laser as a function of delay time, and (b) normalized decay kinetics at 400nm[3]

APPLICATION EXAMPLE: BEHAVIOUR OF CYANOCOBALAMIN IN EXCITED STATES

A second exciting usage of TAS was published by a team at the University of Michigan while studying how cyanocobalamin-excited states behave in biological systems[4]. In this study, they used an Avantes spectrometer to measure how different solvents affect electron transitions, as shown in Figure 6 (next page). The team then used this data to verify a complex quantum mechanical model that they developed to 'lay the groundwork for detailed studies of a range of cobalamin cofactors proposed for use as anti-vitamins, photoactivated drug delivery agents, and in situ production of hydroxyl radicals[4].

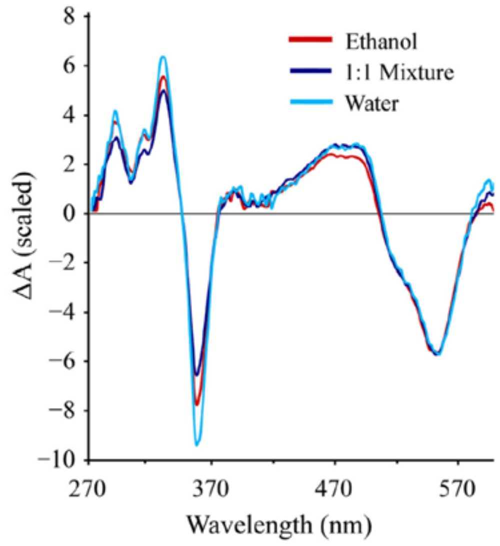


FIGURE 6:
TAS spectra of CNCbl in water, ethanol, and a 1:1 mixture of water and ethanol. Excited with a 266 nm pump laser[4].

APPLICATION EXAMPLE: PHOTOREDUCTION OF GRAPHENE OXIDE

Lastly, a joint team from the Max Planck Institute, University of Hamburg, University of Ioannina, and University of Toronto used TAS to gain a better understanding of photoreduction of graphene oxide[5]. In their study, they used TAS to show that the photoreduction process was actually a multistep process by observing that there were two overlapping decays, one which took place in under 2 picoseconds (ps) and a second taking place between 2ps and 250 ps. The fast decay correlated to the ionization of the graphene oxide and the water-producing solvate electrons, which then interacted with the graphene oxide to cause the reduction during the slow-decay period. The data shown in Figure 7 was collected using an Avantes fiber-coupled spectrometer and excited using 266 nm pump laser.

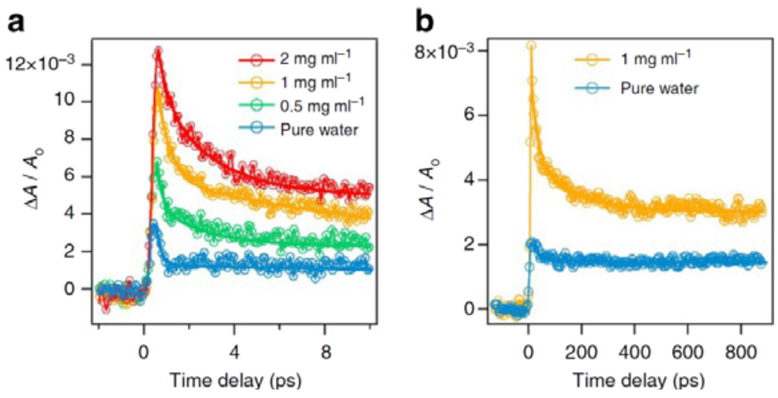


FIGURE 7:
Short-term (a) and long-term (b) kinetic decay of photo-reduced graphene oxide in water using a 266nm pump and the differential absorption at 400nm[5]

FINAL THOUGHTS

As researchers continue to probe more in-depth into the underlying physical chemistry of complex systems like the ones mentioned, it is becoming ever more critical to understand the internal transition kinetics within molecules and atoms.

While this application note is by no means a comprehensive review of the entire field of ultrafast transient absorption, it provides an introductory overview of the physics behind TAS as well as typical system configurations. Furthermore, TAS spectroscopy is currently undergoing a second renaissance with the recent invention of the attosecond pulsed laser, for which Gérard Mourou and Donna Strickland were awarded the Nobel Prize in 2018. Avantes is excited to keep providing the community with cutting-edge spectrometers for the next generation of ultra-fast spectroscopy.

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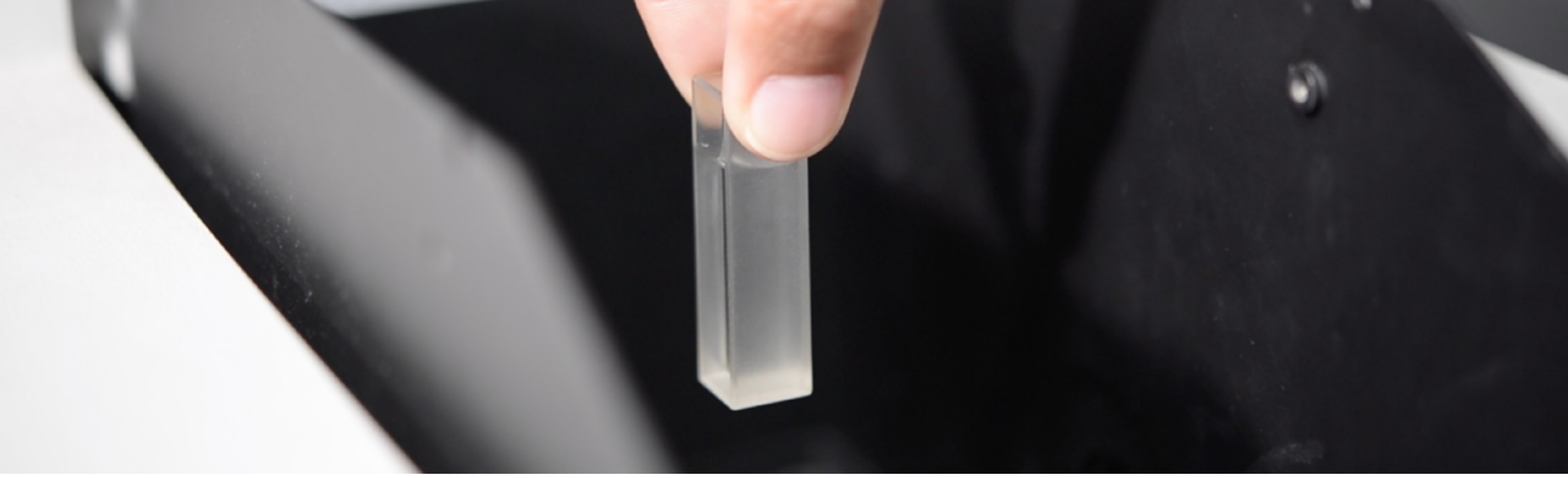

2.7

UV/VIS Spectroscopy Applications in Chemistry

UV/VIS spectroscopy, or spectroscopy in the ultraviolet and visible ranges of the wavelength spectrum, is one of the common tools in many chemists' toolboxes. This versatile measurement technique has a secure place in the chemistry lab. The Beer-Lambert law, which relates the attenuation of light to properties of the material the light is passing through, states that the absorbance of a sample is directly proportional to the concentration of the absorbing analyte. You can frequently see this axiom at work in analytical chemistry to quantify analytes, monitor processes, and reactions, and detect certain organic compounds.

ATMOSPHERIC CHEMISTRY

Atmospheric chemistry plays a central role in our understanding of the mechanisms of local climate conditions and factors into global radiative balance as well. Researchers study a class of compounds called Secondary Organic Aerosols (SOAs) which are the reactive products of gas-phase photooxidation of both naturally occurring and man-made volatile organic compounds (VOCs). There have been many studies on the reaction mechanisms in the propagation of SOAs, Dr Kun Li and a team of fellow researchers from the Institute of Chemistry at the Chinese Academy of Sciences and the Beijing National Laboratory for Molecular Sciences looked more closely at the optical properties of these aerosols under varying reactive conditions[1].

The scattering and absorptive properties, the direct components of the refractive index are more dependent on the composition of the aerosols than of the concentration or particle size. Understanding the link between the chemical composition of aerosol pollutants and their optical properties allows for a more accurate estimate of global radiative effects of localized reactive conditions.

Dr Li's team's work tested the optical properties of SOA particles generated in a Teflon smog chamber in the lab from several different precursor compounds and under varying NOx levels. Using the AvaSpec-ULS2048L-EVO, the particles were shown to be non-absorbent at wavelength 532 nm. Retrieving Refractive Indices (RI) for each sample at that wavelength yielded values ranging from 1.38-1.59, depending on which precursor compound generated the SOA and under what concentration of NOx, but independent of the concentration of SOA or of particle size. Ultimately, their work suggests that many environmental models may overestimate the Refractive Index, and in turn the global radiative effects.

COLLOIDS AND NANOPARTICLE

One area of study in chemistry that has received much attention is Nanoparticles. These nano-scale particles are between 1 and 100 nm in size and surrounded by interfacial layer of ions, organic, and inorganic compounds that can react with other substances. Nanoparticles can exist as a powder or in a solid matrix but are often found in colloidal form, dispersed in an aqueous solution or gel.

Nanoparticles are formed by either breaking down larger particles or by a controlled chemical reaction assembly process. These microscopic particles can be used for molecular tagging, DNA probes, gene therapy, and even cancer treatment. They are found in consumer products such as sunscreens, anti-glare/non-scratch eyeglasses, anti-microbial or heat resistant coatings, and even in food. The processes of chemical assembly of nanoparticles can be temperamental and the stability and reproducibility of a reaction is dependent on many factors, including solution temperature, humidity, and the purity and concentration of the reagents. Any study of nanoparticles necessarily begins with their production and one of the most widely accepted means of reaction monitoring is UV/VIS spectroscopy.

A group of researchers in the Department of Physics at the Kaunas University of Technology, Lithuania analyzed colloidal silver nanoparticles created via silver salt reduction. The chemical reduction of the silver salt solution was monitored throughout the reaction process using the AvaSpec-ULS2048L (now AvaSpec-ULS2048CL-EVO) in the 300-700 nm wavelength range. Colloidal silver exhibits a wide absorption band from 350-550 nm with an peak at 445 nm. As nanoparticles begin to form, absorption increases. As the particles then grow in size, the absorption peak shifts toward the red wavelengths. Stabilization of the absorption peak indicates that new nanoparticles have ceased forming. The data collected during the reaction process also allowed the researchers to calculate average particle size [2].

HUMIDITY DETECTION

Another group of researchers from the School of Chemistry and Chemical Engineering at the Beijing Institute of Technology studying Nano-Hydrogel Colloidal (NHC) array photonic crystals for the detection of humidity, relay on UV/Vis spectroscopy during the precipitation polymerization synthesis process of developing their NHCs. The novel design of this colloidal gel humidity sensor allows the water-absorbing properties of this hydrogel to swell and change volume in response to environmental stimulus. As the particles swell, the change in the size of the particle causes a shift of the absorption bands toward the red. This displays as a change in color visible to the naked eye and tunable, covering the full visible wavelength range from 400-760 nm corresponding to a 20-99.9% range in humidity. These experiments, supported and verified using the AvaSpec-ULS2048LTEC spectrometer (now replaced by the AvaSpec-ULS2048X64TEC-EVO), may lead to new sensor technologies which can be applied to a variety of organic and inorganic molecular detection sensors[3.]

COMPLEMENTARY MEASUREMENT METHODS

While UV/VIS spectroscopy is a powerful tool on its own, this technique is often used in combination with other techniques. The use of complementary techniques can provide researchers with richer data than either technique can achieve on its own. Alternatively, these methods can serve as an accuracy check, with data deviations between methods pinpointing sampling discrepancies.

UV/VIS SPECTROSCOPY WITH ATTENUATED TOTAL REFLECTION (ATR)

Another technique that is frequently paired with UV/VIS spectroscopy is attenuated total reflectance (ATR). In analytical chemistry, where ATR techniques with strongly light-absorbing or optically dense material, can yield data about a sample by exploiting the electromagnetic evanescent field. During ATR, a beam of IR light is passed through a crystal with a high refractive index. Once the sample is in contact with the crystal, the incidence beam reflects off the interior surface of the crystal in contact with the sample. An electromagnetic field generated by the vibrations of this reflection penetrates the sample, revealing a band of absorption where the evanescent wave is attenuated.

Dr. Thomas Bürgi of the Department of Physical Chemistry at the University of Geneva, Switzerland, pairs ATR with UV/VIS absorbance measurements to study oxidation reactions at the point of catalytic interfaces at an in-depth molecular level. During experiments, Dr. Bürgi collected simultaneous and synchronized ATR and UV/VIS spectra. Changing reaction conditions yielded complementary information from the combination of measurement techniques. Attenuated total reflection (ATR) was used with the AvaSpec-ULS2048CL-EVO to identify dissolved reaction products, while UV/VIS spectroscopy was highly sensitive to changes of the catalyst[4].

UV/VIS SPECTROSCOPY WITH RAMAN & ATTENUATED TOTAL REFLECTION (ATR)

Studying the synthesis of mixed oxide catalyst precursors, Dr. Ursula Bentrup and a team of scientists at the Leibniz Institute of Catalysis in Germany used multiple methodologies during their experiments, in order to gain a deeper understanding of how varying synthesis parameters affect the structure and crystallinity of the precursors and the performance of the resulting catalysts.

The in-situ UV/VIS measurements were used in the monitoring of chemical reactions to track the formation and extinction of reactant species. Paired with Raman, researchers could track changes at an atomic scale, revealing a gradual crystallinity change of Co2+ from octahedral to tetrahedral. Using the AvaSpec-ULS2048CL-EVO with a specialized ATR probe, researchers observed absorption bands for molybdenum at 838, 879, 930, 1442, and 1632 nm, as well as a nitrate band around 1338 nm, become broader and more intense as precipitate formation increased. This combined method of investigation has a high potential for real-time monitoring of complex reactions in the liquid phase, including the precipitate of solids[5].

As nanoparticles begin to form, absorption increases. As the particles then grow in size, the absorption peak shifts toward the red wavelengths. Stabilization of the absorption peak indicates that new nanoparticles have ceased forming. The data collected during the reaction process also allowed the researchers to calculate average particle size [2].

UV/VIS SPECTROSCOPY WITH RAMAN & ATTENUATED TOTAL REFLECTION (ATR)

One technique that is often combined with UV/VIS Spectroscopy is Nuclear Magnetic Resonance. German researchers publishing in the journal Angewandte Chemie studied the efficacy of combined UVNMR methodology in reaction monitoring to gain insight into the acid-based chemistry of strongly hydrogen-bonded complexes in aprotic solutions [N*]. These slow reactions are highly sensitive to concentration, temperature, and the solvent used. Using the AvaSpec-ULS2048CL-EVO spectrometer for UV/VIS spectroscopy allowed the researchers to monitor reaction states through changes in the spectra surrounding the phenol group absorption bands found at 315 nm in low pH solutions and shifting to 400 nm in high pH solutions. Meanwhile, simultaneous use of NMR methods yields insight into the hydrogen geometry of the reaction product[6].

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3

SECTION 3

INSTRUMENTS FOR CHEMISTRY APPLICATIONS

There are an unlimited number of applications in the field of chemical spectroscopy. Chemical reactions are dynamic processes that vary with changing conditions which result from various types of techniques. Our instruments are equipped to handle those different applications.

We strive to offer you the best measurement solutions that matches your application needs. Can't find what you are looking for? Contact us, we are happy to help.

3.1 AvaRaman Bundles

Avantes joined forces with two different partners to offer three convenient Raman bundles, consisting of a high-performing spectrometer (three different models), a unique laser-probe combination (785nm) supplying enhanced signals, and an outstanding software package to analyze the Raman spectra.

BUNDLE OPTIONS

There are 3 different bundles, each set-up contains a dedicated spectrometer to your application requirements. The 3 bundles explained:

BUNDLE FOR EXCITATION: AvaLaser785 (incl.: 785 nm laser safety goggles). It has an ultra-high-throughput integrated Raman probe. This novel device includes an integrated wavelength stabilized laser source with Raman filter packs, beam shaping optics, and high-efficiency Raman spectra collection optics.

Features:
- 785 nm Wavelength stabilized excitation source.
- High throughput optical design with 100cm-1 Cut-on.
- External control box for power adjustment (manually/software controlled).

BUNDLE FOR ANALYSIS: AvaSoft-Raman: Basic standalone software to obtain spectra. Panorama-Light: Panorama Light is a modular, high-end software platform for spectroscopic data evaluation. The application meets all requirements for a comprehensive spectroscopy working environment, offering:

- Measurement with an instrument
- 2D & 3D data visualization
- Searching in libraries
- Archiving in spectral libraries, including additional information
- Printing with professional print templates
- Conversion of many known data formats
- Sharing data with office applications Panorama Light is designed to assist you and to keep you focused on work.

BUNDLE FOR DETECTION: We offer state-of-the-art spectrometers based on the StarLine and SensLine, tailored for optimum performance in the Raman range of interest.

3.2 Fluorescence Measurement Options

In spectroscopy, fluorescence is one of the more challenging setups due to the height of fluorescent emission (about 3% of the excitation energy). We show you the best available options for fluorescence measurements below. Click on the name of the products to visit the product page on our website for more information.

SPECTROMETER

AVASPEC-ULS2048CL-EVO

- Grating VA (350-1000 nm)
- 200 µm slit
- DCL-UV/VIS-200 detector collection lens

LIGHT SOURCES

AVALIGHT-HPLED

- Compact LED light source
- High power levels for excitation
- Several excitation wavelengths available

AVALIGHT-XE-HP

- High power fiber coupled 6W pulsed Xenon source
- Perfect for fluorescence
- Easy to integrate

FIBER OPTIC

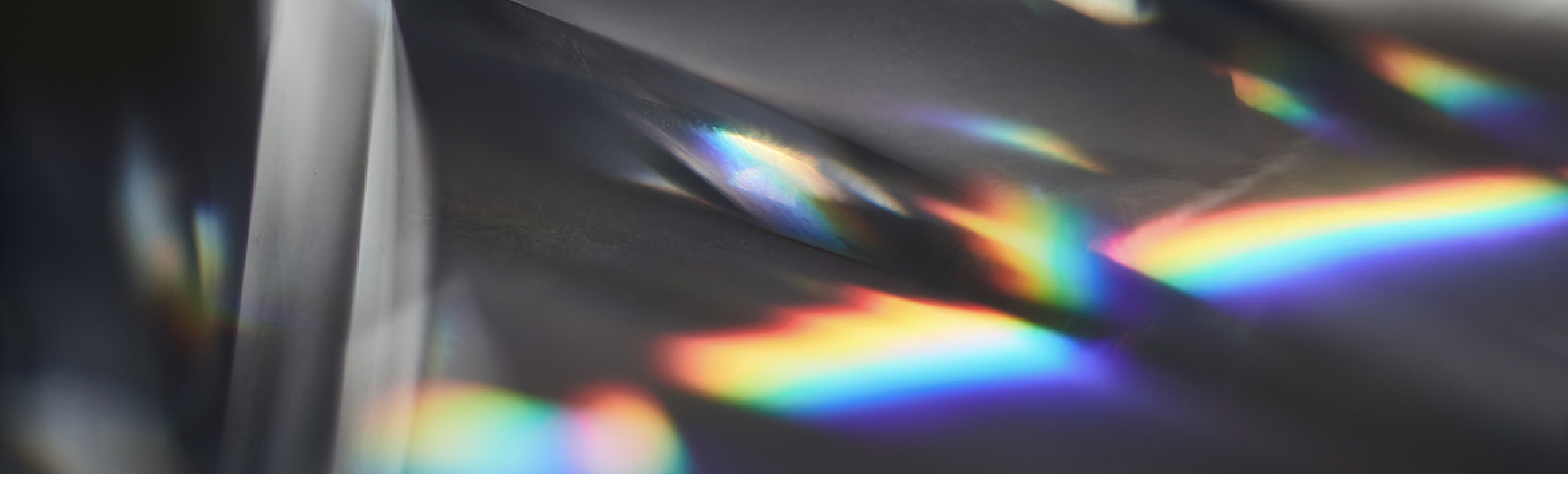
FIBER OPTIC WITH PROBE

- With 600 micron fiber
- Probe for fluorescence
- Surrounded by 12 200 micron excitation fibers

ACCESSORY

DIRECT ATTACHED INLINE FILTER HOLDER

- Two versions available
- For optical separation of excitation/emission signals
- Hold 0.5 inch filters with thickness of 1 to 8 mm



3.3

AvaSpec-ULS2048 x64TEC-EVO

AVASPEC-ULS2048X64TEC-EVO

This instrument enhances the SensLine series with its cooled, back-thinned detector. The back-thinned detector has a high level of sensitivity in the UV and IR region. The 64-pixel height (0.89 mm) enables catching as many photons as possible while the cooling enables long integration times up to 120 seconds with low-noise levels.

It features a Peltier cooling device that is integrated into our ultra-low stray-light optical bench, which can reduce the temperature of the CCD chip to -30°C against ambient, significantly improving the dark baseline and PRNU level. The detector cooling also reduces the dark noise by a factor of 2-3. It uses a special low-noise version of the 2048×64 detector with integrated cooling.

All the features mentioned above make this instrument ideally suited for measuring low-light applications, such as fluorescence or low-light Raman measurements.Optimum flexibility is guaranteed with the replaceable slit.

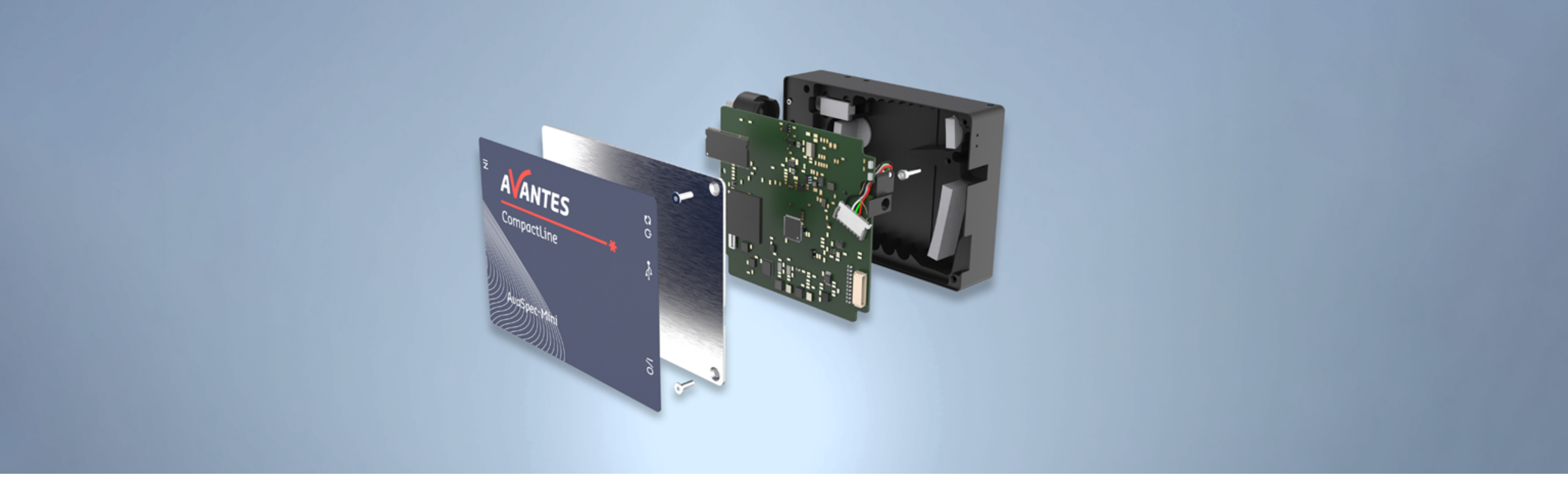
3.4

AvaSpec-HERO

AVASPEC-HERO

Our "HERO" spectrometer is built with High-Sensitivity, Compact (HSC), 100mm optical bench offering a NA of 0.13 and a cooled, back-thinned detector (1024×58 pixels). Electronics wise, it uses our latest AS7010 board, which includes a high-performance Analog to Digital convertor with excellent noise performance and the ability of high-speed communication through USB 3.0 and Ethernet.

The combination of these two state-of-the-art components will give you an excellent instrument, offering the ideal balance between sensitivity and resolution and the capability of using longer integration times in low-light applications, yet ensuring perfect signal-to-noise performance, transferred by the latest communication standards.



3.5 The Compact Yet Powerful; AvaSpec-Mini

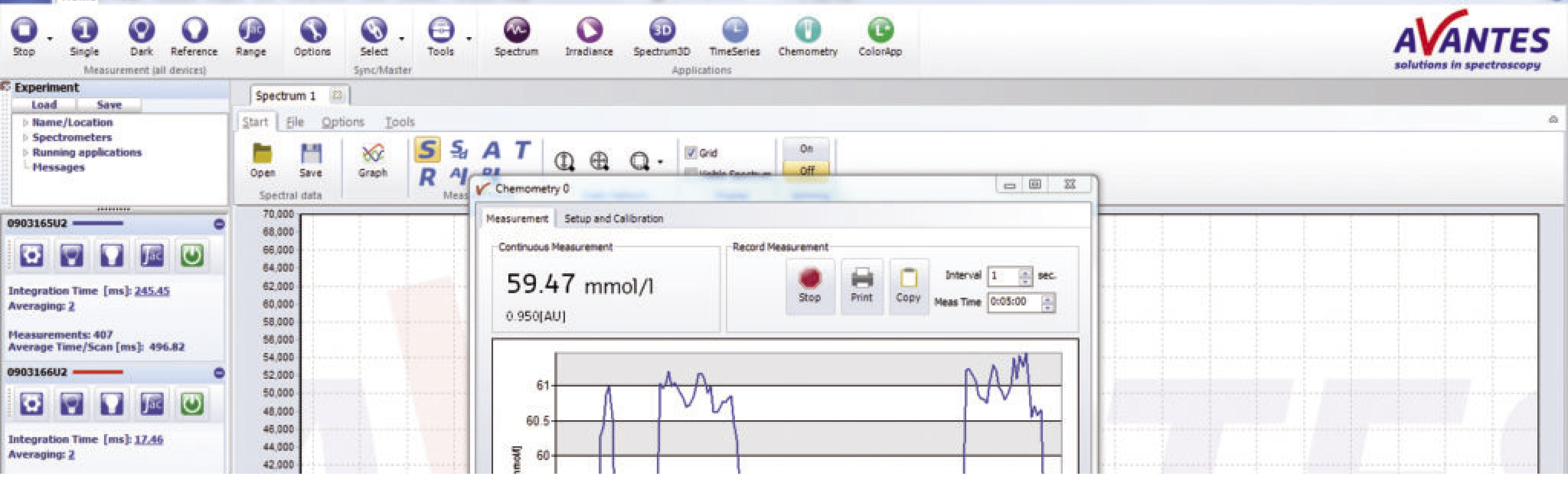
AVASPEC-MINI

Customers wishing to perform chemical spectroscopy in the field often prefer a smaller form factor instrument and Avantes has this covered with our AvaSpec-Mini2048CL, AvaSpec-Mini4096CL, and AvaSpec-Mini-NIR.

The AvaSpec Compactline is a small form factor instrument line that can easily be integrated into any number of field applications. This instrument family features two UV/VIS models (Mini2048CL/Mini4096CL) for 200-1100 nm and one near-infrared model (900-1700 nm).

All Minis are available with a variety of slit sizes, order suppression filters, and other options. The Minis feature USB2 communication and have a 9 pin I/O connector to facilitate external triggering and digital/analog input/outputs.

The Mini has been used in a number of chemistry applications as a desktop or field instrument, but it is primarily designed as an OEM module for integration into customers' systems for applications ranging from chemical process control through biomedical testing.



0903165U2

Integration Time [ms]: 245.45
Averaging: 2

Measurements: 407
Average Time/Scan [ms]: 496.82

0903166U2

Integration Time [ms]: 17.46
Averaging: 2

59.47 mmol/l
0.950[AU]

Interval 1 sec.
Meas Time 0:05:00

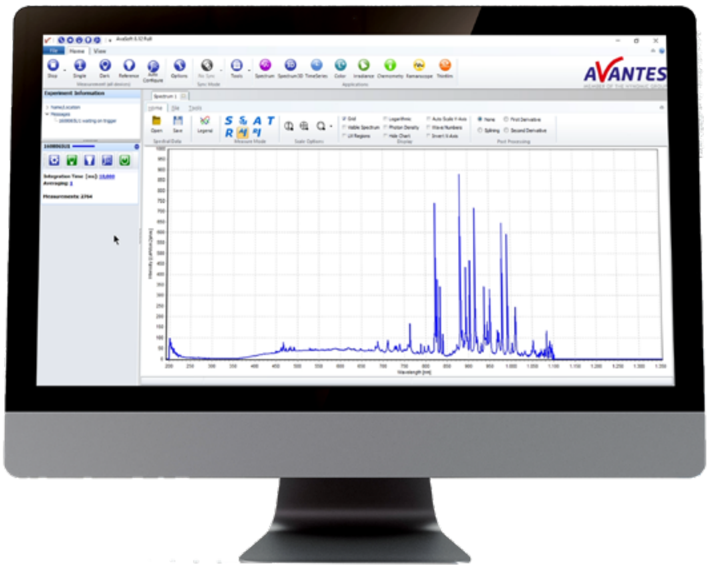
3.6 Software for Chemometry: AvaSoft-CHEM

AVASOFT-CHEM MODULE

The AvaSoft-CHEM module enables online concentration determination with a spectroscopy system. Lambert-Beer's law states there is a linear relationship between absorbance and concentration:

A = e * c * l

Where A is the absorbance (or extinction), e is the extinction coefficient of the compound to be measured, c is the concentration and l is the optical path length. In practice, this relation is only linear at reasonably low absorbance levels (less than 2 Au). To measure the absorbance, a few samples with known concentration are needed. It is important to always measure the absorbance at the same wavelength, and using more samples of different concentrations provides a better chemometric model.



The absorbance values are used in AvaSoft-CHEM to create a linear (or second order – quadratic) calibration line. This calibration line is then used to measure the concentration of unknown samples or to measure the change in concentration over time.

AvaSoft-CHEM can display and save the calculated concentration in the following ways:

- Online display of concentration in a separate display window
- Up to eight history channel functions can be selected to display and save concentration values against time. This application can be combined with the Process-Control applications.

4

SECTION 4

OUR DEMO PROGRAM

4.1 Try before you buy

We understand the importance of getting it right when making an instrument purchase decision. Sometimes applications have special needs that are not known in advance. Our demo program allows you to test an spectrometer, light source, and even some accessories in your experiment or operation to validate functionality and fine-tune specifications. Vetting our instruments in your applications ensures you will be successful after you make a purchase. In the rare event, we don't meet or exceed your measurement demands, we eliminate the need for costly returns and reworks.

4.2 Compare with an Existing Instrument

Often our customers have experienced a competitive or different class of instrument and would like to have a comparison to see if their measurements can be improved or cost-optimized. Demanding applications such as fluorescence and Raman are often performed with high-cost instrumentation which may be overkill for the needs of the applications. Our instruments raise the bar of performance such that our more affordable technology can replace higher cost, slower systems.

4.3 Fine Tune Software Integration & Control

Our demo program allows you to familiarize with our software or take a closer look at our software development kit (SDK) and sample programs. Our instruments can be controlled using our proprietary software AvaSoft or via your own software written in Labview, Matlab, C#, C++, Visual Studio, Python, or any of a variety of Linux environments.

AVANTES
MEMBER OF THE NYNOMIC GROUP

CONTACT

WE'RE HAPPY TO HELP

Curious how spectroscopy can help you reveal answers by measuring all kind of materials, in-line, at your production facility, in a lab or even in the field? Please visit our website or contact one of our technical experts, we're happy to help you.

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