Ocean Optics

Application Note

Keywords

- Gumball sorting
- Color characteristics
- UV-Vis and NIR spectroscopy

Techniques

- Diffuse reflection spectroscopy
- Raman analysis
- Absorbance and transmission
- Oxygen and pH sensing

Applications

- Process monitoring
- Quality control
- Chemical analysis

Operation Gumball: The Sweet Science of Spectroscopy

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In-line gumball sorter demonstrates range of spectroscopy techniques

Consider the simple pleasures of the humble gumball: all the satisfying chewiness of bubblegum and the pleasant crunch of a hard-candy shell, in a sugary, bite-sized sphere. And gumballs aren't just tasty – they're fun, too. A familiar childhood rite of passage involves dropping coins into the arcade gumball machine and excitedly awaiting the sweet goodness inside – and maybe even a prize – with each turn of the handle. Even when you lose, you win.

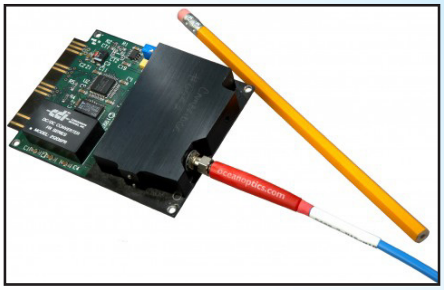

Figure 1: World's First Miniature Spectrometer

For Ocean Optics, developer of miniature fiber optic spectrometers and optical sensing technologies, gumballs have become an ideal – and unexpected – media for demonstrating the power and possibilities of optical sensing technologies. And all it took was a high profile trade show, a lot of ingenuity and a bit of Rube Goldberg-like whimsy to help illustrate the connection.

Our story begins in the 1990s, when Ocean Optics introduced the first miniature fiber optic spectrometer (Figure 1). This modular, compact instrument offered researchers and developers across various disciplines and industries a convenient and affordable complement (and in some cases, alternative) to less flexible, more expensive laboratory spectrometers. Because selling the concept of "miniature modularity" in spectroscopy was new, the need to display the spectrometer in action at trade shows was obvious; prospects could then see what they had trouble believing.

The World's Most Unusual In-line Gumball Sorter

For folks in the photonics industry, the SPIE Photonics West Conference and Exhibition is the most important show of the year, an opportunity for the 20,000-plus exhibitors and attendees to forge new business ties, discover new technologies and showcase the best in new products and services. For Ocean Optics, the 2013 show provided several challenges: to demonstrate a range of spectroscopy techniques, from Raman analysis to reflection measurement; to convey the company's ability to provide solutions for lab researchers, OEMs and industrial customers; and to accomplish all those things and still have fun. The answer: a mechanized in-line gumball sorter.

Figure 2: Gumball sorter setup

Despite its fanciful look – even Willy Wonka would take notice — the Ocean Optics gumball sorter is a sophisticated system comprising multiple spectroscopy measurement stations positioned throughout an 8-foot-tall, 6-sided structure. A series of stainless steel rails mounted to the structure delivers the samples to each station, where spectrometer setups determine gumball sample characteristics such as chemical composition, color and reflectivity (Figure 2). Additional stations around the 900-square-foot booth measure absorbance and fluorescence of food coloring and flavorants, transmission characteristics of plastic containers and oxygen content in packaging headspace.

At the top of the booth, a large hopper holds a collection of 3,000 gumballs (both sugar-rich and sugar-free) and marbles, which look remarkably similar to the gumballs. In traditional gumball fashion, bright reds, greens, yellows, blues and oranges provide a splash of color. Each of these sample characteristics provides an opportunity to sort the samples using fiber optic spectroscopy. As the samples are released from the hopper, they feed through a gravity-driven system of stainless steel rails to their stations. Each station acts as a sort of pass-fail analyzer: a measurement is made and the result registers the response in software, which then triggers a second device – a motorized gate – to direct the sample to the appropriate destination (Figure 3). But less important than the logistics of the booth display are the range and flexibility of the spectral sensing techniques it presents.

Experimental Conditions: NIR Diffuse Reflection

Figure 3: Gumball station (close-up of gumballs after sorting)

Gumballs and marbles are composed of very different materials, yet their similar sizes, shapes and colors make them difficult to distinguish by sight alone. In our gumball sorter setup, we used NIR diffuse reflection spectroscopy to separate gumballs from marbles. In this application, the NIR approach focuses on capturing the distinct reflection intensity differences for each sample's coating and avoids trying to detect slight color differences that one would observe with a visible spectrometer.

For our experiment, we used a NIRQuest512 spectrometer, which is a 512-element InGaAs array spectrometer with response from 900-1700 nm. The setup also included an HL-2000 tungsten halogen source for illumination and a 400 µm fiber optic reflection probe, positioned at 45°, for sample collection.

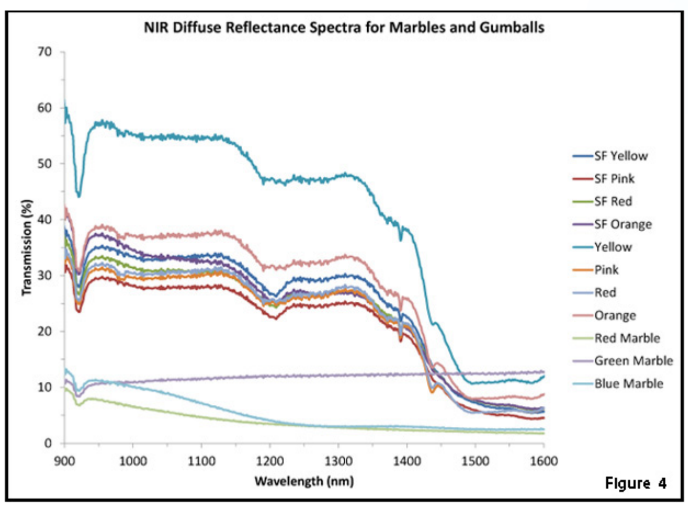

Figure 4: Gumball versus marble spectra

The gumball sorter NIR setup was quickly and accurately able to sort red, blue and green marbles from gumballs, based on differences in reflectivity. The marbles are glossier and have a higher degree of specular reflectivity, resulting in lower diffuse reflection intensity relative to the gumballs (Figure 4). As evidenced by the spectral features in the gumball spectra, additional information on the chemical composition of the samples including sugar and moisture content could be extracted from the spectra using the appropriate chemometrics models. Rejected marbles were binned separately and the gumballs continued through the sorter for further analysis.

Experimental Conditions: Raman for Chemical Analysis

Raman spectroscopy is a very useful technique for determining chemical composition, especially because of the strong specificity of the Raman signature of many materials. In our gumball sorter, we use a modular Raman spectrometer setup to distinguish sugar-rich from sugar-free gumballs. Samples were captured in a Raman sample holder equipped with a Raman fiber optic probe. Excitation light was provided by a 785 nm laser and the Raman spectrum was collected with a QE series back-thinned CCD spectrometer.

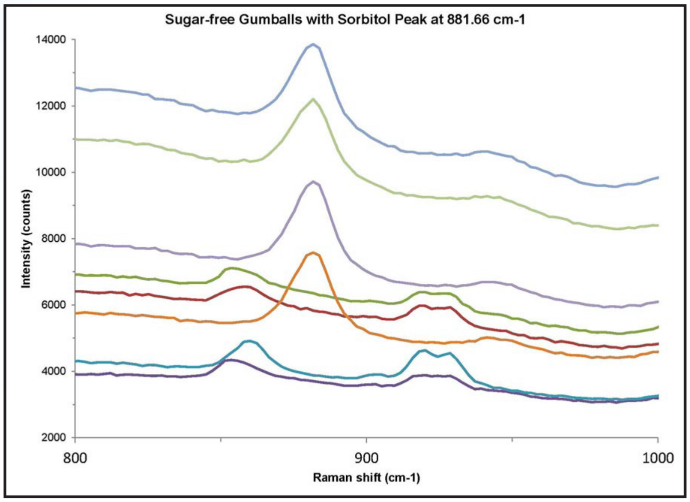

Figure 5: Spectra of sugar-free gumballs with Sorbitol peak

The QE series spectrometer was configured with a 1200 line/mm grating blazed at 750 nm, in an optical bench with an uncooled, NIR enhanced back-thinned CCD array detector. The sugar-free gumballs have a distinct Raman shift near 881 cm-1 that corresponds to the peak for sorbitol (Figure 5), a sugar alcohol often used as a sugar substitute in diet foods and sugar-free gum.

Using NIR excitation light for Raman spectroscopy at 785 nm minimizes fluorescence signals, which dramatically simplifies chemical identification and fingerprinting. Raman is also useful for quantifying mixtures like gumballs (the coating and the gum inside have different chemical composition), as even minor spectral differences are discernible. In addition, Raman can capture data from a sample contained in plastic or other materials (like packaging) that are optically transparent to the wavelengths of interest.

Experimental Conditions: Reflected Color of Sugar-rich and Sugar-free Gumballs

Small-footprint modular spectroscopy systems are readily configured for quality control experiments such as verification of color and appearance of raw materials and finished goods. With our gumball sorter setup, we used three experiment stations to demonstrate the flexibility in design approach that's available with sensing tools for color measurement.

The sugar-rich gumball color station was anchored by the Torus, a concave holographic grating spectrometer distinguished by its low stray light and high thermal stability performance. The Torus has a CCD array detector and was configured with a variable line spacing grating with 550 (+/-2) grooves/mm density at center and the blaze wavelength at 400 nm. An HL-2000 tungsten halogen source for illumination and a 400 µm fiber optic reflection probe for sampling collection completed the setup.

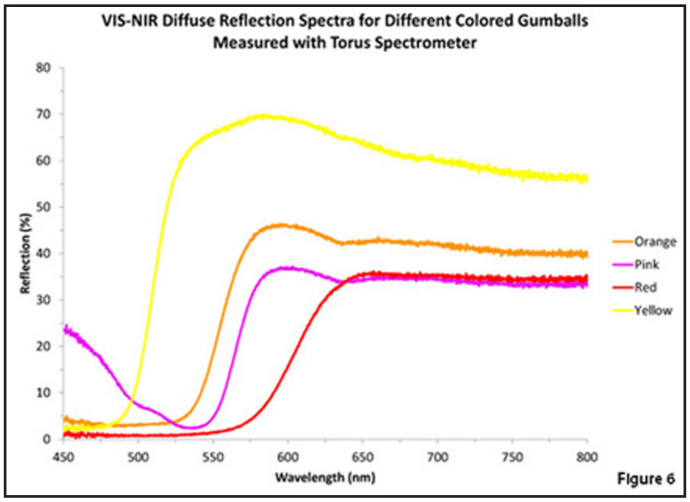

Figure 6: Measurement of color of sugar-rich gumballs

In the Torus setup, the color of the sugar-rich gumballs was easy to observe, although there is visible variability from gumball to gumball (Figure 6). This variability is deduced as being a result of batch differences in manufacturing (a "close enough" standard is probably all the manufacturer was aiming for), fading of the coating color with exposure to air and light, and some "bleed-over" of colors from adjacent gumballs as they collide while moving through the sorting process.

For analyzing color in sugar-free gumballs, we utilized a USB2000+ linear CCD-array spectrometer with an HL-2000 tungsten halogen source for illumination and a 400 µm fiber optic reflection probe for sampling collection. The USB2000+ is one of the most commonly deployed miniature spectrometers in the world and is remarkably flexible, making it more easily implemented into process streams and optimized for all sort of applications. To maintain the temperature of the USB200+ optical bench with changing ambient temperature conditions, the spectrometer was temperature stabilized using a USB-TC temperature controller. The USB-TC stabilizes the bench to within 0.1 °C, providing exceptional repeatability and performance.

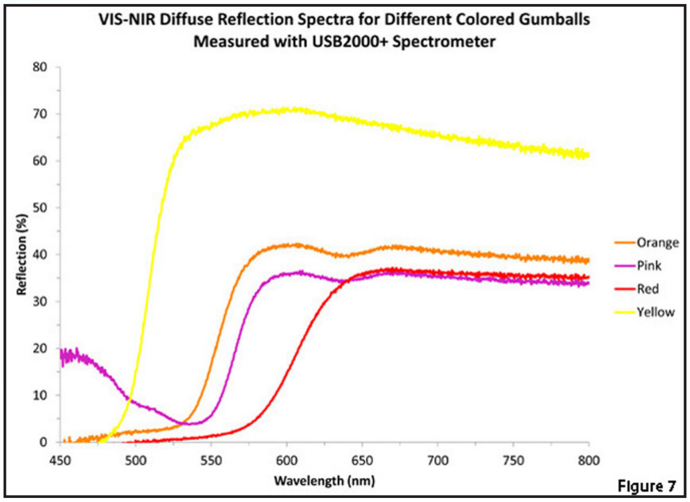

Figure 7: Measurement of color of sugar-free gumballs

In the USB2000+ color setup, the spectrometer was set with a 600 mm-1 groove density grating covering the 350-850 nm range and a 25 µm entrance aperture for good resolution. Similar to what we observed in the results for sugar-rich gumballs, the relative color characteristics of the sugar-free gumballs were readily apparent. Interestingly, the color of coatings for the sugar-rich and sugar-free gumballs revealed differences in relative intensity that varied from color to color (Figure 7). Further analysis would be required to determine the cause of the differences. Also, quantitative color measurements could be performed to sort the gumballs using both Torus and USB2000+ spectrometers that have been properly calibrated for absolute irradiance.

We also used color measurement to demonstrate an "at-line" measurement. As the gumballs exited the process stream, they were collected into containers based on color and sugar content, for additional color QC. Here we performed a spot check of gumball color using the STS microspectrometer, a CMOS-detector device notable for its small size (1.6" x 1.7" x 0.9" LWH), high signal to noise (>1500:1) and great optical resolution (~1.5 nm FWHM). A tungsten halogen source and reflection probe completed the setup.

The STS achieved similar results as the Torus and USB2000+ in measuring relative color. What's particularly interesting about the STS is the performance it delivers for a device its size, which is ideal for embedding into process streams or OEM devices where one or more wavelengths are being monitored and a highly reproducible result is desired.

The Significance of Gumball Sorting

Although our simple gumball sorter isn't designed for high throughput manufacturing or very likely to end up on a factory floor, every instrument in the display and each spectroscopy technique it demonstrates can today be implemented into a process stream, used in a lab or field setting or incorporated into another sensing device. In fact, miniature spectroscopy is especially suited for process environments, where monitoring of incoming raw materials and in processes and finished goods is critical. Flexibility in detectors, light sources and sampling optics allows for deeper implementation of instrumentation into the process stream, and makes it much simpler to optimize setups.

Another consequence is that multiple-point sampling and redundant sensing are easily integrated into on-line applications. In fact, small-footprint modular systems can be rapidly configured for a variety of absorbance, reflectance and emission measurements, with potential applications as far-ranging as monitoring of dye baths for carpeting, analysis of chemical dissolution processes for pharmaceuticals production and verification of color and appearance of (you guessed it) gumballs.

Ocean Optics also manufactures optical oxygen and pH sensors for use in applications in life sciences, pharmaceuticals, biotechnology, food and beverage processing and more. Compared with traditional electrochemical sensing techniques such as galvanic sensors, optical sensors can be made in small and customizable form factors, allow non-intrusive measurements and do not consume the sample.

In the gumball sorter display, we placed oxygen-sensitive adhesive patches inside the gumball product packaging. By introducing canned, compressed air into the package, we were able to show the oxygen sensor's ability to monitor oxygen non-intrusively through packaging. The oxygen content of the packaging is a key indicator of how well the package prevents oxygen from penetrating the space, which can lead to food spoilage or affect food quality.

The limitations of electrochemical-based oxygen and pH sensing are overcome by Ocean Optics optical oxygen and pH patches. Such patches can be integrated within process systems and provide continuous, non-intrusive monitoring of key system parameters. The ability to monitor DO and pH in real time without perturbing a sealed environment can lead to an improved understanding of production processes and help to maintain product quality and safety.

The Sweet Smell of Success

Industrial sensing customers value reliability, ease of use, convenience and productivity. As people get smarter about how they manage their processes, demand has grown for more flexible and less expensive solutions – an "Ocean Optics gumball sorter" approach, if you will — to solving a host of application challenges.

Multi-wavelength spectroscopic sensing – especially in the UV and Visible – has dramatically decreased in cost in recent times when considered on a per-measurement basis. Miniature spectrometer systems can be custom configured and are often much less expensive than traditional benchtop instruments. Furthermore, these systems add flexibility so that reworking them for a changing process is not a particularly expensive proposition. Ocean Optics has sold more than 230,000 spectrometers based on the notion that components and accessories can be mixed and matched easily and inexpensively, without sacrificing performance.

Of course, cost is just one driver. Today's industrial markets demand optical-sensing instrumentation that is more reliable, versatile and adaptable than ever. Already Ocean Optics has worked with hundreds of customers facing those same types of challenges as they tackle the sorting of LEDs, or the manufacture of semiconductor chips or the monitoring of food safety.

And that's a pretty sweet return on investment.

Contact us today for more information on setting up your spectroscopy system from Ocean Optics.

Ocean Optics

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