Integrated Spectral Sensors

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New approaches that mimic the functioning of the human eye are enabling embedded, portable alternatives to conventional spectrometers.
Color vision is the most powerful tool used by humans and animals to gather biochemical information from objects in their environment. The spectrum of light diffusively reflected from materials is determined by absorption bands related to molecular vibrations and their overtones—spectral bands that occur when a molecule makes a transition from the ground state to higher-order vibrational states. This spectral information, which in human eyes is collected by three types of cone cells with different spectral responses, is processed into the perceived color. That, in turn, provides the remarkable ability to predict biochemical properties of objects from their appearance—for example, to judge the ripeness of fruit, to identify plant stress from the color of the leaves, and to assess the status of a wound.

This information can be made more accurate and quantitative by measuring the spectrum of diffuse reflectance with higher spectral resolution and in a wider wavelength range than eyes can process—a task usually performed by spectrometers. For decades, near-infrared spectroscopy (NIRS) has been used to classify materials and quantify their chemical composition because the first and second overtones of important functional groups and molecules, such as CH, CH₂, CH₃, and H₂O, are located in the NIR part of the spectrum.

Recently, the increasing need for real-time sensing solutions in industrial and agricultural applications, as well as the concept of “embedded spectroscopy” integrated into consumer appliances, have driven the quest for compact, low-cost spectroscopic instruments and advanced methods for extracting useful data from the measured spectra.

While most commercial solutions use a scaled-down version of well-proven spectrometer concepts, approaches are emerging that challenge the conventional wisdom that spectroscopy requires the measurement of a full spectrum. These new “spectral sensors” mimic the operation of human eyes in that they use a very limited set of spectral measurements—a spectral “fingerprint.” As they are easily integrated on a chip, they have the potential to become as ubiquitous as CMOS cameras.

From spectrometry to spectral sensing
The miniaturization of commercial spectrometers has relied mainly on clever designs based on the
workhorse of spectrometry, the combination of gratings and detector arrays. Compact spectrometers involving Fourier-transform geometries, linear variable filters and electromechanically tuneable filters have also been commercially deployed. However, the small size and low costs required for consumer applications can be reached only with wafer-scale integration.

Researchers have dedicated considerable effort to chip-based spectrometers, resulting in a number of ingenious approaches to measurement of the light spectrum, either directly (wavelength by wavelength) or indirectly (through spectral reconstruction). A major practical hurdle, however, is that light from diffuse reflectance is spatially incoherent and cannot be efficiently coupled to a photonic integrated circuit or any other device that operates on a single spatial mode. This greatly limits the number of options for integrated spectrometers that measure the full spectrum—a large number of closely spaced wavelength points.

However, the analogy with human color vision suggests that limited spectral information, the power in few spectral bands, can also enable accurate predictions of important biochemical characteristics—an approach known as spectral sensing. This approach is particularly well suited to NIRS, as the spectral features of reflection or transmission spectra of most organic materials are relatively broad.

Conceptually, a spectral sensor, also known as a multispectral sensor, consists of an array of detectors, each associated with a different filter. Implementations based on discrete detectors and filters have long been used in various sensing applications, such as nondispersive infrared gas sensing. A similar spectral-sensing approach is also employed in pulse oximetry, in which two LEDs with different spectra are used to measure the fraction of oxygen-saturated hemoglobin in blood. However, this approach is difficult to scale to a large number of spectral bands, as it involves packaging and assembling numerous discrete components.

The performance and applicability of such sensors have greatly increased in recent years with the development of integrated arrays of filters and detectors, in which the filter array can be monolithically integrated or co-packaged with the detector array. Filters can be implemented on top of the detectors as multilayers (in the simplest case, a Fabry–Pérot cavity with two Bragg mirrors) working in transmission mode, or they can become an integral part of the detector by placing the absorber in a resonant cavity.

Sensor technologies
This progress in integration has led to the industrial development of spectral-sensing chips consisting of pixels with distinct spectral responses. Their small millimeter-to-centimeter form factor and wafer-scale fabrication make them very attractive for portable and embedded spectroscopy. The combination of the responses of the different pixels can cover a very broad spectral range, for example, from 400 to 1000 nm or 850 to 1700 nm.

In terms of technologies, a clear distinction can be made between silicon-based sensors, which operate in the visible and NIR range up to about 1100 nm, and sensors based on InGaAs or organic photodiodes, which can also cover the NIR range above 1100 nm. Silicon sensors can in principle take advantage of advanced CMOS technology, and in fact RGB image sensors are
The measurement of hundreds of wavelength points with high resolution is not an efficient approach to the sensing problem, as it produces redundant data that must be compressed again.

Regardless of the specific technology used, these sensors do not qualify as spectrometers due to the limited number of spectral points (typically between 8 and 32), the relatively large linewidth (10 to 50 nm) and, in some cases, the presence of multiple peaks or a background. It is therefore crucial to assess how the corresponding spectral data can be used and what level of prediction accuracy can be obtained for relevant applications.

**Making sense of spectra**

To understand the potential and limitations of spectral sensors, it’s helpful to review the approaches used to build predictive models for standard spectrometers (see “Analyzing spectral data,” p. 51). Generally, a model can be built by making a large number of measurements on a set of samples where the parameter of interest—for example, sugar content—is independently measured using a calibrated method. Using these data, a regression model is then constructed to predict the value of the parameter from a spectrum of an unknown sample. Chemometrics is the scientific discipline that investigates these models by data-driven means.

The data from conventional spectrometers typically have a much larger number of observed variables (spectral points) compared with the number of measurements and their corresponding targets (sugar content), and the observed variables are strongly correlated with each other. Robust models therefore cannot be built by directly applying multiple linear regression (MLR) to associate the targets to the full set of intensities at different wavelengths, as this would lead to overfitting—a model too closely aligned with the limited data set used to build the model to make predictions on other data sets.

To avoid this error, the information from the original spectra is usually “concentrated” in a new set of meaningful data with a reduced number of variables. Picking a few significant wavelengths at which the measured intensity of different samples differ most would be the easiest way of reducing the spectra. However, this is not an optimal use of the incoming light and can be very subject to noise at those wavelengths, and the wavelengths for which the spectra

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**Spectral responses of the 16 pixels in a near-infrared InGaAs spectral sensor.** The detectors were integrated within a Fabry-Perot cavity, forming a resonant-cavity-enhanced photodetector, and the spectral response is varied by changing the thickness of the cavity. The peaks cover the 900–1700 nm range and have a linewidth of 50–60 nm.
A wide variety of methods has been developed to deal with these issues, of which partial-least-square (PLS) analysis is a prominent example. In PLS, the full data consisting of spectral points are projected to a new basis, for which the covariance between the new predictor, consisting of latent variables (LVs), and target is maximized. The LVs are linear combinations of the observed variables that best model the targets, and the spectral weights represent the weights of each observed variable on the LVs.

In practice, this means that the wavelengths where the measured spectra vary the most for different values of the quantity of interest will have more weight in the underlying LVs. As a result, only a few LVs are required to capture most of the relevant information from the spectra. Also, for solid materials the spectral weights of the LVs—their expression in the wavelength basis—mostly do not show narrow features, indicating that high spectral resolution is not needed. This clearly indicates that the measurement of hundreds of wavelength points with high resolution is not an efficient approach to the sensing problem, as it produces redundant data that must be compressed again.

### Using data from spectral sensors

When samples are measured using a spectral sensor instead of a spectrometer, the resulting data have fewer points, or observed variables, which are less correlated due to the discrete spacing of the wavelength bands measured by each pixel. In some cases, the data points acquired by a spectral sensor can be directly used in MLR for prediction of the target. In

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**Analyzing spectral data**

Process for analyzing data obtained from spectrometers, using the example of sugar content in a tomato.

1. **Collect the data.** Reflectance spectra of tomatoes with varying sugar content, showing spectral features related to absorption by molecular transitions. Data: G. Polder, Wageningen University & Research

2. **Use partial-least-square (PLS) analysis to get the latent variables (LVs).** Spectral weights of the two dominant LVs. A large positive or negative value in a given band indicates a strong correlation with the target parameter [sugar].

3. **Regress the first variable to assess fit.** Value of the first LV versus measured sugar content. The LV already shows a reasonable correlation with the sugar content, but it is far from optimal ($R^2$ of 0.52).

4. **Improve the fit by boosting number of LVs.** Predicted versus measured sugar content using 14 LVs. Using multiple linear regression, a better predictor can be built using additional LVs, resulting in a more robust prediction model ($R^2$ of 0.98).
this direct regression using sensor data, measurements from a subset of pixels are often highly weighted in the MLR due to their high correlation with the quantity of interest.

However, depending on the number of pixels in the sensor and their spectral response, directly applying MLR to the sensor data can still result in overfitting and suboptimal modeling. The prediction performance can often be improved by optimizing the way that spectral information is captured and used in a regression model, for example, by the use of PLS analysis.

The process described above has a close connection to compressive sensing: The measurement is not done on the basis of the wavelength but on the basis of the filter functions defined in the sensors. It is therefore not critical that the filters show a single peak or very high off-band suppression, as long as they can probe the spectral variations in the sample. Also, while reconstructing the incoming spectra from the photocurrents may be possible, it is not useful, as it expands the data set without adding information.

As mentioned above, most solid materials are in principle suitable for characterization with spectral sensors due to the absence of narrow spectral features. The type of sensing problem—and particularly whether the spectral bands measured by the sensor match the spectral weights of the samples—determines whether spectral sensors can provide a prediction accuracy competitive with the one of standard spectrometers and what spectral range is most useful.

Real-world uses

Our team has recently demonstrated several practical applications of a prototype 16-pixel InGaAs NIR spectral sensor: detection of fat content in milk; classification of plastic types; and classification of drugs. In the first example, calibrated milk samples with varying fat content were measured by the sensor, housed in a handheld module, in reflection mode. To model the fat content using normalized absorbance values from the sensor measurements, PLS was used to reduce the 16-dimension pixel data to LVs, of which only four were used to build the prediction model. The model's performance on unknown test data achieved a high R² value of prediction of 0.98 and a small RMS error of prediction of 0.15%.

In the plastic classification experiment, 90 samples consisting of PET, HDPE, LDPE, PP and PS (both the rigid and foam types) were measured in reflectance. PLS was applied to transform the normalized absorbances, and 10 LVs were used as input to a discriminant analysis (DA) classifier for predicting the plastic type. The PLS-DA model obtained an accuracy of 100% in the prediction of unknown test set samples.

In the drug classification example, 11 types of high-purity substances ranging from illicit to common household drugs were measured: MDMA, amphetamine, caffeine, cocaine hydrochloride, cocaine base, heroin, ketamine, levamisole, lidocaine, methamphetamine and paracetamol. The samples were crushed into powder form, sealed in glass vials and measured in reflectance. In this case, the chemical fingerprint measured by the spectral sensor was sufficiently unique to each drug type and modeling was done using DA directly. The model was able to accurately distinguish between the various sample types with 100% accuracy.

The future of spectral sensing

The above examples show just a glimpse of the potential of integrated spectral sensors. In the short term, they
Ultimately, the wide deployment of spectral sensors and the corresponding increase in production volume will drive down their fabrication costs. can be used for process monitoring in the chemical and agrofood industries and for material classification purposes in the recycling sector. An upcoming, high-volume market is embedded spectroscopy in household appliances and wearables. Ultimately, integration into smartphones will provide the largest market opportunities—in fact, visible-range spectral sensors are already included in high-end smartphones for color and ambient light sensing.

In addition to directly measuring the properties of materials from their reflected spectrum, spectral sensors can also be used to indirectly measure a property of interest through the spectral response of a transducer, such as a colorimetric sensor. This affords the possibility of measuring low concentrations of analytes that would not be detectable in the absorption spectrum—for example, trace molecules in liquids or gases—and thereby opens a much wider range of applications in environmental sensing and biomedical diagnostics.

New applications will also drive further advances in the technology. On one hand, increasing the number of pixels and reducing the linewidth of the sensor leads to improved spectral resolution and may help improve sensing accuracy. However, this comes at the cost of lower signal per pixel and increased complexity of the readout, and it also puts tighter specifications on the wavelength accuracy and the numerical aperture, due to the angular dispersion of the filter. It is therefore expected that spectrometers will remain the solution of choice for problems requiring resolutions of much less than 10 nm.

On the other hand, a considerable gain can be obtained by extending the spectral range. Combining visible and NIR sensitivity (400–1700 nm) in one multiband sensing module, if not one device, would allow much more freedom in selecting the relevant spectral signatures for different problems. Extending to the 1.7–2.3 μm band—which would be possible using using extended InGaAs photodiodes, for example—would be significant, as spectral signatures of relevant chemical bonds are present in the first-overtone and combination regions. Further extension to the mid-infrared is possible, but it would require other materials, detection principles or both and possibly cooled operation.

Ultimately, the wide deployment of spectral sensors and the corresponding increase in production volume will drive down their fabrication costs. This is a consequence of wafer-scale fabrication methods and a key difference with conventional spectrometer technologies based on discrete components, which require more complex packaging and assembly. Eventually, integrated spectral sensors could provide consumers with a powerful tool for chemical analysis embedded in household appliances, wearables and smartphones.

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References and Resources


For acknowledgements, go online: optica-opn.org/link/spectral-sensing.
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