Miniaturized Short-Wavelength Infrared Spectrometer for Diffuse Light Applications

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Abstract: A miniaturized short-wavelength infrared spectrometer for use with diffuse light was created by combining a thin form factor carbon nanotube composite collimator, a linear variable filter, and an InGaAs photodiode array. The resulting spectrometer measures 3 x 4 x 14 mm and shows a significant improvement in resolution over a spectrometer without the collimator when used with diffuse light. Its small size and high throughput make it ideal for applications such as wearable optical sensing, where light from highly scattering tissue is measured. Plethysmographic measurements on the wrist were demonstrated, showing rapid data collection with diffuse light.

1. Introduction

Recent advancements in tissue measurements have enabled the widespread use of wearable health monitors. These monitors incorporate sensors to obtain and report a wearer’s physiological data, with the goal of enabling more informed health decisions. More versatile miniature sensors can provide additional physiological information1, 2. One region of the optical spectrum with untapped potential for continuous measurement of physiological information is the short wavelength infrared (SWIR)3, 4, which typically incorporates 900-1700 nm light. In this region, there are key absorption peaks for biological molecules such as glucose, urea, triacetin and water3, 5, 6. However, changes in these peaks cannot easily be isolated using traditional broad LEDs and a single photodiode, causing them to become confounding variables for one another. This presents the need for higher resolution data, a challenge that may be addressed by a miniaturized spectrometer.

Spectroscopy is an invaluable tool in better understanding materials and the chemical makeup of matter7, including physiological concentrations of molecules. SWIR spectroscopy has been applied to many fields including: tissue classification8, food quality9, soil testing10 and recycling11. Recent research has been focused on both miniaturizing and reducing the cost of spectrometers to increase their availability and utility12-16. Spectrometers use various methods to separate the light into composite wavelengths, including: diffraction gratings17, wedge filters18, Fourier transform19, metasurfaces20 and tunable filters21. Each technique requires collimated light for optimal performance. Wedge filter-based spectrometers, which operate on the same principle as thin-film interference band pass filters have been studied as one route to spectrometer miniaturization18, 22-24. In a wedge filter, the interference layer thickness varies from one side to the other across the filter. This results in a passband center wavelength that varies with position. When the allowed wavelengths change linearly along the wedge, the filter is called a linear variable filter (LVF). When an LVF is combined with a linear photodiode array, each pixel in the array correspond to specific wavelengths resulting in a simple spectrometer18, 25.

LVF’s resolution is highest when incoming light is collimated perpendicular to the surface of the filter. However, after passing through tissue, outgoing light is highly diffuse3. This presents a challenge for LVF-based spectrometers as the detected light is no longer perpendicular to the surface of the filter26. Other miniaturized spectrometer approaches also require collimation for high-resolution measurements. A collimator could be used to collimate the light prior to the spectrometer, but traditional lens- or aperture-based collimators require long optical...
pathlengths, making them non-ideal for miniaturized devices. One solution to this issue is to utilize parallel hole filters, a type of collimator that can be miniaturized. Parallel hole filters are densely packed arrays of high aspect ratio tubes that geometrically limit light transmission to a small range of angles around normal incidence. I.e., off-axis light will pass through one end of the tube and be absorbed in the wall of the tube but on-axis light will pass down the axis of the tube and exit the other side. With the aid of carbon nanotube templated microfabrication (CNT-M), we recently designed, fabricated and tested a miniaturized collimator intended for spectrometer-based wearable optical monitoring. CNT-M based collimators have a fairly simple fabrication process and naturally result in absorptive surfaces, they offer a significant reduction in size compared to traditional lens collimation, allowing miniaturization beyond what is currently on the market.

In this work, we present the design and characterization of a miniaturized SWIR spectrometer for diffuse light applications. Without the need of a grating or lenses, the spectrometer size was reduced to 3 mm x 4 mm x 14 mm. The spectrometer consists of a CNT-M collimator, an LVF, and a 128 pixel linear photodetector array (figure 1). The resulting resolution (Full Width Half Max-FWHM) of 13 nm at 1300 nm and the collimating characteristics are compared to an analytical optical model. The dark current noise was measured to be -28dB. Additional calibrations, including dark current subtraction and bright field correction, are discussed in the supplemental document. In a human subject experiment, the sensitivity of the miniaturized spectrometer was compared to a commercially available grating-based spectrometer (size: 88.9 mm x 63.5 mm x 31.9 mm) and found to have a throughput more than 100x higher. Using surface-mount light emitting diode (LED) illumination, the spectrometer was used to demonstrate the collection of high quality plethysmographic signal from the radial artery of the wrist.

Figure 1) Schematic view of the spectrometer assembly. A) Monochromatic diffuse light enters spectrometer from the top. The light is collimated by the CNT collimator, separated by wavelength by the LVF and ultimately collected by the photodetector array. Compare spectrometer (B) compared in size to a quarter. A 3D printed holder contains the linear variable filter and collimator and is sealed with a plastic window. The Photodiode array is attached to a flexible substrate. Full spectrometer is compared to the size of a quarter. C) CAD illustration of the collimator, LVF and Photodiode array. This exploded view shows the components without the 3D printed holder.

2. Materials and Methods
The carbon nanotube collimator was manufactured using the CNT-M process as described previously\textsuperscript{27, 29, 30}. Briefly: 70 nm of alumina was reactively sputter-coated onto silicon substrates. A carbon nanotube (CNT) growth catalyst (4 nm of iron) was then deposited in a pattern onto the substrate using contact lithography, thermal iron evaporation and liftoff. Carbon nanotube forest growth with ethylene gas was performed on the catalyst-coated silicon substrates in a one-inch tube furnace at 750 °C. The growth time was 6 minutes to achieve the desired CNT growth height of 400 µm. Following growth, the CNT forest was infiltrated with carbon (10 minutes in ethylene at 900 °C) to improve the strength of the CNT-M collimator. After growth and infiltration, the samples were exposed to an oxygen plasma for 10 minutes to remove excess carbon deposited on the substrate during infiltration and release the collimator from the substrate. CNT-M fabrication uses common semiconductor processing tools and as such would not be cost prohibitive in relation to more complicated part such as the LVF or photodiode array.

The spectrometer was assembled using the CNT-M collimator, a linear variable filter (Viavi Solutions) and a photodiode array (Hamamatsu G13913-128FB). All single spectrum data collection measurements from the Hamamatsu array were made using a development board and software provided by Hamamatsu. A 16-bit microcontroller-based (Teensy 3.5) data collection system was developed and used for longer runs and pulsatile data collection and was described previously\textsuperscript{31}. The collimator housings were designed using computer-aided design software (CAD) and 3D printed on the Formlabs Form 3 stereolithography printer using Formlabs standard black resin (Supplemental Document) To protect the collimator during spectrometer handling, a thin glass or plastic slide was cut and attached to the collimator housing using super glue. A CAD model of the assembly is shown in figure 1C (for illustration the housing is not shown).

The spectrometer was constructed with dimensions of 3 mm x 4 mm x 14 mm and is shown in figure 1B alongside a U.S. quarter for scale. In this configuration, the spectrometer is connected to a flexible PCB for ease of testing, but it can also be directly mounted to a printed circuit board (PCB). Figure 1C shows a CAD model of an exploded view of the spectrometer, with the three main components arranged from top to bottom: the collimator, LVF, and photodiode array.

The resolution of the spectrometer was determined using the setup illustrated in figure 2B. Monochromated light was provided by a with a tungsten filament light source and a monochromator (Spectral Products DK240), with a calculated spectral width of 2 nm based on the slit width used. Light exiting the monochromator was diffused using a diffusing mirror (Thorlabs DG10-1500) reflected onto a 100 degree engineered diffuser that was placed directly on the spectrometer (figure 2B). Diffused light illuminated the full spectrometer, and the full width half max (FWHM) of the beam was measured. Resolution was measured every 100 nm starting at 1000 nm and ending at 1500 nm, both with and without the collimator, to determine its effect on spectral resolution and overall performance. The monochromatic light was dim and required an integration time of 0.5 s to get a clear signal. Dark current was collected by taking a spectrum when the illuminating light source was off and subtracted from each spectrum. Wavelength calibration was done by mapping photodetector pixels to monochromator center wavelength values, with linear interpolated values used for pixels between peaks\textsuperscript{32}.

To calibrate for the varied pixel-to-pixel responsivity, brightfield correction was performed by illuminating the spectrometer with a broad-spectrum tungsten halogen bulb. The collected spectrum was smoothed using a 5 boxcar average. Each pixel from the smoothed spectrum was divided by the same pixel in the raw spectrum to get a gain correction ratio. This ratio was divided into future spectra as a bright field correction. This process and the associated uncertainty is discussed further in the supplemental document.

To characterize dark noise, dark current was measured in a temperature-controlled chamber for over 20 hours. The charge from each pixel was converted to a voltage and all 128 pixels were recorded every 10 ms by the microcontroller. The 10 ms cycle time consisted of an 8.5 ms charge integration time and a 1.5 ms data readout time for the 128 pixels. The dark current noise was measured to be 6 A/D counts (-28 dB) and is plotted in the supplemental document. The temperature dependence of the spectrometer dark current signal was measured by varying the chamber temperature in a controlled manner from 0-40°C while collecting data with the non-illuminated spectrometer. This yielded a change of up to 1000 A/D counts, with the data shown and discussed further in the supplemental document. The smoothing effect of brightfield and dark current corrections and their associated uncertainties on a spectrum is demonstrated and further discussed in the supplemental document. Typical signals are 10’s of thousands of counts so 1000 count dark levels are small but not ignorable. Data processing substracts these dark levels. The spectrometer has been studied under a small range of normal operating conditions with no
anomalous temperature effects. However, extreme temperature impacts on efficiency of optical path or photodiode response have not been studied.

**Human Subjects Measurements**

A human subject wrist-based test was performed to compare the throughput of the miniaturized spectrometer to a small commercially available grating-based SWIR spectrometer (Ocean Insight Flame NIR). The comparison measurement was a transfectance measurement on the wrist from a broadband tungsten source to the spectrometer. The tungsten source consisted of a 100-Watt tungsten bulb coupled to a 12mm diameter, 3-ft fiber optic bundle. The fiber optic bundles from the tungsten source and the Flame spectrometer were placed adjacent to each other on the skin of the wrist approximately above the radial artery. A spectrum was collected using the Flame’s automatic integration feature which selected an integration time of 5500 ms. The Flame was then replaced by the miniaturized spectrometer at the same spacing and light intensity and the experiment was repeated with an integration time of 30 ms, chosen to yield similar A/D counts across the spectrum.

Pulsatile measurements were performed using the miniaturized spectrometer coupled with LEDs (Marktech 1206 SMDs) in a single unit. Five LEDs were used with center wavelengths of 1050 nm, 1300 nm, 1550 nm and two at 1650 nm. The LEDs were arranged linearly along the side of the spectrometer to locate them near the corresponding pass-band wavelength locations on the LVF, approximately 4 mm away from the edge of the LVF. The spectrometer was placed on the wrist with the detector above the radial artery and the LEDs on the nearest tendon side of the artery. Once positioned over the artery, neither placement nor pressure was altered to optimize pulsatile amplitude. Data collection was performed using the microcontroller-based system using an integration time of 8.5 ms with complete spectra collected every 10 ms for approximately 3 minutes. Human subjects research in this study was done with approval from the institutional review board at Brigham Young University (IRB #F2020-268).

### 3. Theory

Linear variable filters can be modeled as a series of Fabry-Perot filters, which are thin film interference filters used to isolate a narrow spectral band of light. The spectral pass-band is determined by the space between two thin films mirrors, creating a cavity for resonant wavelengths to pass through. These filters are designed for collimated light to enter at near normal incidence. When diffuse light is used, the filter loses selectivity, allowing a much larger band of light through (Figure 2A). When incident light is off normal, the pathlength of light is lengthened, allowing out of band wavelengths to pass. The CNT-M collimator limits higher angle incident light from passing to the LVF thus retaining the wavelength selectivity of the LVF. Figure 2A shows the effect of a 100-µm wide collimator pore with varying heights (Also see Supplementary Information).

The model we use to calculate filter transmission combines three components: normal incidence transmission through a Fabry-Perot cavity, the change in effective wavelength in the cavity due to angled incident light, and the limiting of angles by the collimator based on aspect ratio. Figure 2A shows predictions of the model with no collimator and then with collimators of varying aspect ratios.

The Fabry-Perot cavity model uses double reflectors separated by a gap with the assumption that the angle does not exceed the critical angle where light would be totally reflected. Transmission through a Fabry-Pérot filter at normal incidence given in Equation 1. \(^3\) In our calculations, we use incident light that is unpolarized with a hard cut-off in angle at ±50°.

\[
T_{\text{tot}} = \frac{T_{\text{max}}}{1 + F \sin^2 \theta}
\]

\[
\theta = \frac{4\pi n_{\text{filter}} d}{\lambda_{\text{vac}}}
\]
$T_{\text{tot}}$ is the total light transmitted through the filter, $T_{\text{max}}$ is the max transmission possible by the filter (set to 50% based on minimum transmission given by manufacturer), $F$ is the finesse coefficient calculated based on the specifications given of the filter (FWHM of about 1%), yielding a value of ~1000. $n_{\text{filter}}$ is the index of refraction of the filter, it was assumed to be 1.33 as it was not provided by the manufacturer. $d$ is the thickness of the cavity (distance between reflectors), and $\lambda_{\text{vac}}$ is the wavelength of light incident on the filter in a vacuum. This equation assumes normal incidence transmission. The index of refraction and thickness of the cavity are a half integer multiple of the expected pass-through wavelength ($n_{\text{filter}}d$ was set to the pass-through wavelength). In practice, LVFs include additional step filters to block wavelengths of nearby half integer multiples of the pass-through wavelength. For simplicity, these multiples are ignored in this model and the wavelengths graphed in figure 2 are limited to our range of interest, which does not include these higher multiples.

With angled (off-normal) incident light, wavelengths longer than the normal incidence filter pass band are transmitted. This out-of-band transmission degrades resolution, as seen in the no collimator and low-aspect-ratio collimator plots in figure 2A. Angled light results in an “effective” cavity wavelength that is shorter than the actual light wavelength. Equation 2 maps the actual wavelength $\lambda_{\text{center}}$ at incident angle $\theta_{\text{in}}$ to an effective pass-through wavelength $\lambda_{\text{eff}}$. $\lambda_{\text{eff}}$ is used to replace ($n_{\text{filter}}d$) in equation 1 to calculate angled light transmission.

$$\lambda_{\text{eff}} = \lambda_{\text{center}}\left(1 - \frac{1}{n_{\text{filter}}\sin^2(\theta_{\text{in}})}\right)^{1/2}$$

(2)

The collimator impacts transmission in two ways. First, it causes shadowing loss due to decrease in open area. I.e., the collimator walls block a fraction of the light from passing even at normal incidence. Second, it reduces
the allowed angles that can pass through the collimator. This is determined by geometric optics and the aspect ratio (ratio of height to pore width) as shown in equation 3. The higher the aspect ratio, the more limited the allowed angles that can enter the LVF.

\[
\theta = \arctan\left(\frac{\text{pore width}}{\text{height}}\right)
\]

\[\text{(3)}\]

4. Results

The spectral resolution of the spectrometer was characterized with diffuse light to simulate the high level of scattering that occurs when measuring body tissue. Tests were performed with and without collimation to show the collimator’s effect on the spectral resolution. The collected spectrum shown in figure 2C is from illumination by a narrow wavelength band light source centered at 1300 nm and diffused prior to detection by the spectrometer. The transmission is shown without a collimator (plotted in orange dots) and with a collimator (plotted in blue dots), with model predictions added for comparison. The amplitude and baseline offset for the model were fit to the measured data using a fitting method of determining the scalar for the amplitude that minimizes the distance between the data points and the model (Lines). The no collimator and with collimator data sets match the model at the center wavelength with a sharp transmission peak. The no collimator measured data set exhibits the same features as the model with the sharp peak at the center wavelength and an additional right-sided tail. The baseline of the result without a collimator is much higher than that of the collimator measurements and the theoretical model. The measured no collimator results also have peaks at the edges of the spectrum not shown in the model. With the collimator in place, the peak decreases rapidly and no other features are detected; the resolution of the spectrometer matches that specified by the LVF manufacturer 1% of the pass-through wavelength or 13 nm at 1300 nm.

To test resolution at multiple wavelengths the center wavelength was varied in 100 nm steps from 1000 nm to 1500 nm and the resulting collimated spectra are shown as dots in figure 2D. Model predictions are plotted in solid lines and the amplitude and baseline offset of the model were fit to the data. The resolution of the spectrometer was measured by determining the FWHM when the collimator was in place (figure 2D). The data for the longer wavelengths (1200-1500 nm) have similar intensities and a resolution of about 1% of the center wavelength. The measured intensities of the 1000 nm and 1100 nm peaks are lower than those of the longer wavelengths. The baseline signals of the measurements all seem to increase near the 900 nm side of the spectrometer, which may be due to a small light leak on that side of the LVF.

A tissue transfectance measurement was performed using the miniaturized spectrometer in comparison to a commercially available grating based SWIR spectrometer. The spectra from two spectrometers, when illuminated on the wrist, were collected at different integration times to show the differences in throughput in a wearable application. The resulting data are shown in figure 3. To obtain similar A/D counts as measured on both spectrometers, the grating based spectrometer had an integration time of 5500 ms while the miniaturized spectrometer had an integration time of 30 ms. The grating based spectrometer’s spectrum is significantly noisier, likely due to the long integration time. No bright or dark field corrections are applied to the miniaturized

Figure 3). Spectrum measured on the wrist with both a grating based SWIR spectrometer and our miniaturized spectrometer. The integration time was varied to get the same A/D counts on both devices. The flame integrated from 5500ms while the miniaturized spectrometer integrated from 30ms.
spectrometer for this comparison. Although illuminated with a broad light source, both spectra have a large peak at about 1050 nm and a second small peak at about 1300 nm. In the miniaturized spectrometer, there appears to be a peak start at 1650 nm.

Plethysmographic spectra were taken on the wrist with the spectrometer placed over the radial artery and the LEDs on the tendon side on the wrist (Figure 4). An LED board was glued to the 3D printed housing of the spectrometer. A wrist strap as shown in figure 4 was used to hold the spectrometer in place. Cables for the spectrometer and LEDs came out the side of the spectrometer module. Data was collected using the microcontroller for several minutes. A 7.5 second segment of that data, for the 1050 nm pixel is shown in figure 4. The pulsatile variation in the data shown sits on the 51,000-count background shown in the vertical scale.

5. Discussion

The advantage of a CNT-M collimator in a compact spectrometer has been demonstrated both theoretically and experimentally with diffuse light. The chief advantage of the collimator for an LVF based spectrometer is its small size while significantly improving diffuse light resolution. For the spectrometer data shown in figure 2C, the resolution (the full width half maximum, FWHM) improves from ~60 nm without a collimator to ~13 nm with a collimator. This improvement is achieved by allowing a narrower range of angles into the LVF, as the width of the LVF pass-band is smallest for near-normal incident light. The collimator limits off normal incident light by blocking the transmission beyond the collimator cut-off angle, which is determined by the pore size and height of the collimator.

Increasing the aspect ratio of the collimator pores can improve resolution up to a certain point, but reduces light throughput. The Fabry-Perot filter model can help choose the desired tradeoff between throughput and resolution. As shown in figure 2A, peak intensity decreases with collimator height while resolution increases. The model calculates passband width from two factors: (1) the normal incidence resolution inherent to the Fabry-Perot cavity and (2) the angular broadening due to non-normal incident light. For narrower cut-off angles, angular broadening has less impact on resolution. However, below a certain cut-off angle, y further reduction does not improve resolution. This occurs when the resolution is limited by the inherent normal incidence resolution of the LVF. As shown in figure 2A, going from 400 µm to 600 µm (with a pore size of 100 µm) results in a minimal gain in resolution but significant reduction in light throughput. A collimator with a height of 400 µm and pore size of 100 µm, resulting in a cut-off angle of 14.3°, gave the largest throughput without compromising resolution. We called this our optimized collimator.
The resolution of the miniaturized spectrometer with optimized collimator compared well against the inherent normal incidence resolution of the LVF across its spectral range. The LVF specifications give a normal incidence FWHM resolution of <1% of the pass-through center wavelength; we will call this the “LVF limited resolution”. The spectrometer’s resolution at near-normal incidence was measured with non-diffuse light using a krypton calibration source (details in Supplemental Document) resulting in a 13 nm FWHM, matching the LVF specification (e.g., 1% gives 13 nm FWHM at 1300 nm). With diffuse light and the optimized collimator, we showed a resolution essentially matching the “LVF limited resolution” across the spectrometer’s spectral range (Figure 2D).

There was found to be good agreement between the collimation theoretical models and experimental results. Two main artifacts were identified in the transmission data collected without a collimator: a significant baseline signal across the entirety of the spectrum and a sharp rise in signal at the ends of the spectrum, one near 900 and the other near 1650 nm (see figure 2c). Although these artifacts were significantly reduced with the collimator, we will discuss their possible origin. The baseline signal may be due to off-normal incidence light bypassing the LVF (leaking around the sides of it) and illuminating the photodiode array without passing through the filter. The rise in signal seen at the edges of the spectrum may likewise be due to non-normal light leakage around the physical edges of the LVF. The collimator cuts off most off-normal incident light, minimizing these light-leakage based artifacts.

Outside the peak in each spectrum of Figure 2D, the A/D counts exhibit a fairly constant baseline across each spectra (except for wavelengths shorter than 1150 nm). However, there is a drift in this baseline as subsequent spectra are taken. The total drift was about 500 counts from the first to the last. The order of spectra taken was: 1400 nm, 1500 nm, 1300 nm, 1200 nm, 1100 nm, 1000 nm. We attribute the baseline drift to an increase in dark current with temperature as the InGaAs sensor warms up, consistent with the measured temperature dependence of the dark (Supplemental Document). All spectra show elevated current at wavelengths shorter than 1150 nm that increases as we approach the short wavelength edge of the spectrometer. We attribute this elevated current to light leakage around the short wavelength edge of the spectrometer constructed to obtain the comparison data displayed in figure 2. This particular spectrometer was designed with a removable collimator, making it more difficult to control light leakage, but not compromising the comparison.

In human subject testing (Figure 3), our miniaturized spectrometer demonstrated a 100-fold increase in throughput compared to the commercial grating-based IR spectrometer. Grating based spectrometers have built in collimation to allow for use in diffuse light measurements, but result in larger size. We attribute this improvement to the differences in optical components between the two technologies. We do not know the specific innerworkings of the commercial grating-based spectrometer, the loses could be do to the various optical components, including the grating resulting in long integration times (5500 ms) for this diffuse light application. In contrast, our miniaturized spectrometer has fewer optical components and only experiences losses due to the LVF and collimator, allowing for significantly reduced integration times (30 ms). This is particularly important for plethysmographic measurements, where multiple spectra must be collected within a single cardiac cycle.

Our miniaturized spectrometer has demonstrated the ability to collect plethysmographic data by measuring pulsatile waveforms. Despite the relatively small amplitude of the measured pulse compared to the non-pulsatile portion of the signal (600 A/D counts peak-to-peak pulsatile vs ~51000 A/D counts of the non-pulsatile offset), we did not alter placement or pressure to optimize pulsatile amplitude once the spectrometer was placed generally over the artery. The 1050 nm peak was chosen to illustrate the pulse due to its high signal and large pulse, serving as a reference for finding the pulse at other wavelengths with lower signals.

We demonstrated the ability to measure plethysmographic data by collecting pulsatile waveforms with the miniaturized spectrometer. The pulsatile amplitude was relatively small compared to the non-pulsatile portion of the signal (600 A/D counts peak-to-peak pulsatile vs ~51000 A/D counts of the non-pulsatile offset).

6. Conclusions

We have designed and characterized a miniaturized SWIR (900-1650 nm) spectrometer for diffuse light applications. This SWIR spectrometer measured 3 mm x 4 mm x 14 mm. This device is the smallest diffuse light SWIR spectrometer currently available. This small size could allow for more consumer level applications in measuring food quality and soil analysis. By using a CNT-M collimator, the spectrometer can filter out diffuse light and achieve a spectroscopic resolution of 13 nm FWHM at 1300 nm, matching the LVF manufacturer specifications.
Human subject measurements were performed under IRB protocols and showed that the miniaturized spectrometer had a throughput over 100 times higher than a grating-based spectrometer in wrist-based measurements. Using LEDs, we collected a pulse on an individual. Further customization of individual components, such as using thinner glass on the LVF, could reduce its size even more. The quality of physiological measurements made by the miniaturized spectrometer demonstrates its potential for use in wearable configurations to collect biometric data.

**Data Availability:**

Data used to generate information in this paper can be found at github.com/twestover13/Miniaturized-Spectrometer-for-diffuse-light

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