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Design of a miniaturized integrated spectrometer
for spectral tissue sensing

Gebirie Yizengaw Belay1, Willem Hoving2, Heidi Ottevaere1, Arthur van der Put2,
Wim Weltjens2 and Hugo Thienpont1

1Vrije Universiteit Brussel, Faculty of Engineering, Dept. of Applied Physics and Photonics
(TONA), Brussels Photonics Team, B-PHOT, Pleinlaan 2, B-1050 Brussel, Belgium
2Anteryon Optical Solutions B.V., Zwaanstraat 2-A, 5651 CA Eindhoven, The Netherlands

ABSTRACT

Minimally-invasive image-guided procedures become increasingly used by physicians to obtain real-time characterization
feedback from the tissue at the tip of their interventional device (needle, catheter, endoscopic or laparoscopic probes, etc…) which can significantly improve the outcome of diagnosis and treatment, and ultimately reduce cost of the medical
treatment. Spectral tissue sensing using compact photonic probes has the potential to be a valuable tool for screening and
diagnostic purposes, e.g. for discriminating between healthy and tumorous tissue. However, this technique requires a low-
cost broadband miniature spectrometer so that it is commercially viable for screening at point-of-care locations such as
physicians’ offices and outpatient centers. Our goal is therefore to develop a miniaturized spectrometer based on diffractive
optics that combines the functionalities of a visible/near-infrared (VIS/NIR) and shortwave-infrared (SWIR) spectrometer
in one very compact housing. A second goal is that the hardware can be produced in high volume at low cost without
expensive time consuming alignment and calibration steps. We have designed a miniaturized spectrometer which operates
both in the visible/near-infrared and shortwave-infrared wavelength regions ranging from 400 nm to 1700 nm. The
visible/near-infrared part of the spectrometer is designed for wavelengths from 400 nm to 800 nm whereas the shortwave-
infrared segment ranges from 850 nm to 1700 nm. The spectrometer has a resolution of 6 nm in the visible/near-infrared
wavelength region and 10 nm in the shortwave-infrared. The minimum SNR of the spectrometer for the intended
application is about 151 in the VIS/NIR range and 6000 for SWIR. In this paper, the modelling and design, and power
budget analysis of the miniaturized spectrometer are presented. Our work opens a door for future affordable micro-
spectrometers which can be integrated with smartphones and tablets, and used for point-of-care applications. As next steps
in the development, we will manufacture the different optical components and experimentally characterize the spectrometer
device in more detail.

Keywords: Miniature spectrometer, visible/near-infrared, VIS/NIR, shortwave-infrared, SWIR, design, spectral tissue
sensing

1. INTRODUCTION

Minimally-invasive image-guided procedures are becoming increasingly important in clinical practice. In a variety of
procedures physicians lack reliable feedback on the type of tissue at the tip of their interventional device (needle, catheter,
endoscopic or laparoscopic probes, etc…) to ensure they are at the right position before effecting the actual diagnosis or
treatment. Spectral tissue sensing using compact photonic probes has the promise to be a valuable tool for screening and
diagnostic purposes, e.g., for discriminating between healthy and tumorous tissue. Real-time tissue-characterization feedback to the physician during an intervention can significantly improve the outcome of diagnosis and treatment, and ultimately reduces the cost of the medical treatment\textsuperscript{1-5}. Diagnostics by means of spectral sensing is being used in a wide variety of point-of-care healthcare applications, such as photoplethysmography (PPG) sensors, capnometers and pulse oximeters. Also, more advanced spectroscopic applications are being reported in literature and will gradually be adopted in the normal workflow in a hospital. Spectral monitoring can be used e.g., for the detection of skin melanoma\textsuperscript{6}, for localising tumors using fluorescent markers\textsuperscript{7} or for detecting tumor margins during surgical interventions\textsuperscript{8}. Whereas the relatively simple PPG or pulse-oximeters rely on the detection of a few wavelength bands in the visible range, more advanced tissue sensing and screening relies on spectroscopic monitoring of a wide wavelength range, simultaneously covering both the visible and infrared part of the spectrum. Since spectral fingerprints of many molecules relevant for diagnostics and screening extend towards the shortwave-infrared, spectroscopic instruments are required that are capable of measuring the full visible/near-infrared to shortwave-infrared region of the electromagnetic spectrum. Nowadays the major clinical trend is the gradual transition of screening, diagnosis, and treatment from hospital to the point-of-care settings. Where traditionally screening and diagnostics was always performed within the radiology department, in the future mobile, cost-effective imaging and sensing solutions will enable physicians outside of the radiology department to diagnose and treat at the patient bedside, in the general practitioners office or day-clinics, or even in a home setting. This will enable earlier detection of diseases and treatment outside of expensive clinical infrastructures and thus reduce the overall financial burden on the healthcare system. However, here, the enabling factor is the availability of small, affordable and easy to use devices.

The concept of a spectral tissue sensing device is shown in Figure 1. The device contains optical fibres for broad-band light delivery towards the tissue under study and collection and transport of scattered light from the tissue towards a measurement console. The measurement console contains a set of spectrometers capable of analyzing the scattered light in the 400-1700 nm spectral range. From these diffuse reflectance spectra one is able to derive physiological parameters like e.g., blood, oxygenation and lipid content of the tissue that is present in front of the photonic device tip, giving real-time feedback of the tissue characteristics to the physician during the intervention. In order to properly quantify these different tissue parameters, the visible/near-infrared (VIS/NIR) as well as the shortwave-infrared (SWIR) parts of the spectrum contain important molecular fingerprints (see Figure 2), that need to be subsequently recorded\textsuperscript{9}. The spectral sensing technology is being investigated for real-time tissue characterization feedback in image guided procedures such as nerve detection in anesthesiology and as biopsy guidance in oncology, however, it can be also used for several other applications, e.g., food quality monitoring, agriculture, industrial inspection, etc.

![Figure 1. Spectral tissue device, reporting real-time feedback on tissue type, blood oxygenation, etc. to a physician\textsuperscript{10}.](image)

For a widespread use of spectral tissue sensing, broadband miniature spectrometer devices should become available at affordable cost, to make it commercially viable for also screening at point of care locations such as physicians’ offices and outpatient centers. Therefore, the goal of our research is to develop highly-integrated portable spectral-sensing devices covering a broad spectral range across the visible/near-infrared and shortwave-infrared (VIS/NIR-SWIR, 400-1700nm) part of the spectrum\textsuperscript{10}.
This paper is structured as follows. Section 2 describes our approach we proposed to design a miniature spectrometer and reviews the current state-of-the-art of compact spectrometers available in the market. The modelling and design of the miniature spectrometer is explained in section 3. Section 4 is dedicated for the sensitivity and irradiance analysis of the designed miniature spectrometer. Conclusions are drawn in section 5.

2. MINIATURE SPECTROMETER BASED ON DIFRACTIVE OPTICS

Current state-of-the-art spectrometer devices contain two fully-fledged spectrometers inside a unit or just a separate spectrometer which works either in the visible/near-infrared (VIS/NIR) range or SWIR-infrared (SWIR) range. Figure 3 shows current state-of-the-art spectrometers from different vendors.

![Figure 3. Some current state-of-the-art compact spectrometers: (a) the AvaSpec-Mini spectrometer of Avantes, (b) the STS series compact spectrometer of Ocean Optics, and (c) the ultra-compact spectrometer of Hamamatsu.](image)

The AvaSpec-Mini spectrometer of Avantes has a dimension of 95 x 68 x 20 mm\(^3\). It operates from 220 nm to 1100 nm\(^1\). The Ocean Optics STS spectrometers have a dimension of 40 x 42 x 24 mm\(^3\). They are available in some limited wavelength regions, e.g. 350 nm - 800 nm or 650 nm - 1100 nm\(^2\). Whereas the Hamamatsu finger-tip sized microspectrometer is probably the most compact spectrometer device available in the market today. It has a dimension of 20.1 x 12.5 x 10.1 mm\(^3\) and it operates from 340 nm to 850 nm\(^3\), but its resolution of 15 nm is insufficient for the intended application.

The objective of our research is to develop an ultra-compact spectrometer based on diffractive optics that combines the functionalities of a visible/near-infrared (VIS/NIR) and shortwave-infrared (SWIR) spectrometer in a compact housing of typically 1 cubic inch\(^4\). In our research, we investigate a novel design of a micro-spectrometer which combines ease of assembly, cost-efficiency and excellent performance in a small size. Our design strategy relies on utilizing the latest developments in digital camera technology with CMOS and InGaAs image sensors, and a reduction of the number of optical components by function integration. A minimum amount of discrete hardware components (“blocks”) is being used and time-consuming mechanical alignment and calibration procedures are taken over by software routines of which the results are stored in EPROM. Figure 4 (a) and (b) give an overview of today’s technology (left), and our approach (right), respectively.
In our approach the number of components is reduced from five to two/three depending on the type of configuration chosen. This has advantages such as easier assembly of the instrument, more compact systems and a lower total cost. In this concept “we think in blocks” using state-of-the art two-dimensional CMOS-image sensors readily available from the camera industry, and a segmented diffraction grating (see Figure 4 below), optimized for the wavelength range. The result is that we obtain an excellent overall performance of the spectrometer that combines compactness with low cost, a large spectral range and high sensitivity.

Figure 4. Left - Traditional layout of a spectrometer consisting of five separate components that must be accurately assembled and adjusted: 1) a narrow slit at the input, which serves as a point source, 2) a curved mirror (collimator) that makes the incoming beam parallel, 3) a diffraction grating that deflects the colors of the incoming light at different angles (“rainbow” effect), 4) a curved mirror (focusing mirror) that focuses the color spectrum onto a linear detector, and 5) the linear CCD-detector that converts the color information into electrical signals. Right - The number of components is reduced from five discrete parts to two "blocks" that are simply put together, namely the DGM (Detector-Grating-Module, the heart of the spectrometer) and the light entrance slit. Precise adjustment and calibration of the spectrometer is done after mechanical assembly with standard image processing software. There will be a large cost reduction if we miniaturize the spectrometer optics for the combined VIS/NIR-SWIR instrument into an integrated design.

The miniature spectrometer in our approach consists of two spectrometer segments: a visible/near-infrared (VIS/NIR), and a shortwave-infrared (SWIR) segment, respectively. The VIS/NIR segment covers wavelengths from 400 nm to 800 nm and the SWIR segment covers 850 nm to 1700 nm. The gratings of the spectrometer are chosen to maximize the overall diffraction efficiency of the spectrometer device.

### 3. MODELLING AND DESIGN OF A COMPACT VIS/NIR - SWIR SPECTROMETER

The main goal of the design task is to keep the size of the spectrometer as small as possible while satisfying the required resolution, SNR and the other specifications determined by the application. The Numerical Aperture, NA of the spectrometer affects both its resolution and SNR. Large NA means more light power is available for the spectrometer (throughput), however due to optical aberrations the resolution will be low. On the other hand, small NA means less light in the spectrometer but better resolution. Therefore, the NA should be chosen that a good balance is obtained between the throughput and resolution of the spectrometer. The NA of the micro-spectrometer was chosen to be 0.15 which is less than the NA of 0.2 of the input fiber. As a result, 20 % of the light power of the fiber is not collected by the spectrometer, but the resolution is improved by a factor of 2 (compared to resolution of a spectrometer with NA of 0.2).
3.1 Spectrometer configurations

We have investigated in detail two basic spectrometer configurations, the first one using a single concave grating and the other using a flat grating and a spherical mirror as schematically shown in Figure 5. The first configuration where a single concave grating is used, is called the Rowland circle configuration and the second one is called the Fastie-Ebert configuration. The two configurations have a relatively small number of components such that a compact spectrometer can be realized and a decent performance can be achieved. Especially, the Rowland circle configuration has the least number of components, but manufacturing the concave grating on a curved profile is very challenging at least to start with. Therefore, we proceeded with the Fastie-Ebert configuration, it has one additional component compared to the Rowland circle, but the grating can be designed and manufactured on a planar surface which strongly reduces the manufacturing complexity. The interesting aspect of the Fastie-Ebert configuration is that coma aberrations can be corrected by the spherical mirror as the light hits the mirror surface twice: firstly at the top part and secondly at the bottom of the mirror\textsuperscript{14}.

![Figure 5. Two basic configurations for the spectrometer: (a) the Rowland circle configuration with one concave grating, (b) the Fastie-Ebert configuration with a spherical mirror and a flat grating\textsuperscript{14}.](image)

3.1.1 Open arms Fastie-Ebert configuration

As can be seen from Figure 5(b), the disadvantage of the classical Fastie-Ebert configuration is that there is not enough space to position the source (input optical fiber), grating and detector within a cubic inch device. Therefore, the grating was moved forward with respect to the spherical mirror to create extra space between the grating and the source on the one hand and the grating and the detector at the other hand. We call this the “open arms configuration”. Then the grating is positioned closer to the mirror and tilted while keeping the overall size of the spectrometer very compact (Figure 6).

![Figure 6. “Open-arms” Fastie-Ebert configuration for the spectrometer design to create space of the detector.](image)

We have chosen the “open-arms” Fastie-Ebert configuration shown in Figure 6 for the two spectrometer segments. The dimensions of the configuration are shown in Figure 6. The distances between the components are between their respective centers. The radius of curvature of the spherical mirror and the distances between the different components are chosen so that the overall size of the spectrometer configuration remains within one cubic inch, and the different components can be simply put together to build the spectrometer device.
3.2 Design of the two spectrometer segments

The two spectrometer segments, i.e. the VIS/NIR and the SWIR segments have a similar configuration as the basic configuration shown in Figure 6. Therefore, they have the same overall sizes. The only difference between the designs of the segments is the blaze wavelength, grating pitch and spectral range. This results in the same diffraction angle and blaze angle for the grating segments. The grating component of the basic configuration is designed so that the central wavelength of the spectral range will be detected at the center of the detector. This will ensure that the whole spectral range of the two spectrometer segments is collected at the available VIS/NIR and SWIR detectors.

4. ANALYSIS OF THE SPECTROMETER

4.1 Power budget and sensitivity analysis of the spectrometer

A sensitivity analysis of the spectrometer was done to verify if there is enough light available for the spectrometer to operate for the spectral tissue sensing applications. The total amount of light available for each wavelength at the detector is determined by several factors. The most prominent factors are the light source spectrum, the absorption and scattering characteristics of the tissue constituents such as water and hemoglobin, the diffraction efficiency of the gratings and the detector’s spectral response. Moreover, the NA of the spectrometer will affect the spectrometer throughput. To determine the spectrometer NA, a trade-off between the light throughput and resolution of the spectrometer device needs to be made. For the power budget calculation, we assumed a standard halogen light source. According to health and safety regulations, the total power of the light at the probe end to which the tissue is exposed should not exceed 6 mW\textsuperscript{15}. We took a light power of 5 mW in our sensitivity analysis. The absorption characteristics of the tissue constituents such as water determine the amount of light backscattered from the tissue. The backscattered light from the tissue that is collected by the multimode fiber connected to the spectrometer input is about $10^{-4}$ of the incident light power at the probe end close to the tissue. Moreover we have taken into account the diffraction efficiency of the gratings for the two grating segments and the quantum efficiency of the detectors. The two gratings are blazed for at least 60% diffraction efficiency in the range from 400 nm to 1700 nm. For the VIS/NIR spectrometer a CMOS detector from CMOSIS, CMV 4000 (2048x2048 pixels, pixel size 5.5 µm) detector is used\textsuperscript{16}. For the SWIR, an InGaAs linear array (512x 1 pixels, pixel pitch 25 µm, pixel height 250 µm) infrared detector is used for the calculations and the experiments\textsuperscript{17}. The signal-to-noise ratio (SNR) of the spectrometer was calculated taking into account all the above parameters. The SNR of the spectrometer is shown in Figure 7. The SNR is higher than 151 (21 dB) in the VIS/NIR, and 6000 (37 dB) for SWIR. This is enough for spectral tissue sensing in the range from 400 nm to 1700 nm.

Figure 7. SNR of the spectrometer: (a) linear scale, (b) in dB.

4.2 Irradiance analysis of the spectrometer

The latter modelling does not take into account the actual intensity distributions within the light beams. The SNR calculated above for the wavelengths from the different influencing factors (diffraction efficiency, quantum efficiency of the detectors, tissue absorption) are used as weighting coefficients for the wavelengths in CODE V (ray tracing program) to simulate the actual light distribution/irradiance at the detector. The irradiance measures the distribution of light power per unit area, it could be a measure of the light power received per pixel. Ultimately, the irradiance analysis gives us an idea
of the resolution limit of the spectrometer. The resolution of the spectrometer is determined by the FWHM of the irradiance which specifies the difference of two closest wavelengths which still have a non-overlapping irradiance at the detector.

An irradiance analysis has been performed for the two spectrometer segments in their respective spectral ranges taking into account the SNR values for the wavelengths. This allows us to see how the light is distributed over the detector for each spectrometer segment. We then take the cross-section of the detector in the dispersion direction (vertical direction in Figure 8(a)) to see how the light is distributed over the different wavelengths within the spectral range of the spectrometer segment. For the irradiance analysis we assume that the slit acts as a light source having a Gaussian profile. The slit has a width of 25 µm and height of 200 µm. The source is assumed to have a Gaussian beam profile with a width of 200 µm and a NA of 0.2 (or a half divergence angle of 11.54°) using a multimode fiber of diameter 200 µm and NA of 0.2 to collect the light scattered from the tissue and bringing it to the input port of the spectrometer. The irradiance plot of the VIS/NIR spectrometer segment are shown in Figure 8(a). The cross-section of the irradiance is shown in Figure 8(b). We took two wavelengths separated by 6 nm (e.g. 400 nm and 406 nm) in the three regions of the first VIS/NIR spectral range (lower range at 400 nm, middle range at 600 nm and upper range at 800 nm). We then run the irradiance analysis and see if these adjacent wavelengths which are separated by 6 nm, are well distinct or resolved at the detector. The analysis shows that the different colors are well separated, which means they are spectrally resolved. In Figure 8(a) we see separated lines in the different regions of the detector indicating that the 6 nm resolution is achieved. Also from the cross-sectional plot in Figure 8(b), it is seen that the different peaks are well distinct which assure us that the 6 nm resolution has been achieved with simulation.

![Irradiance plots](image)

Figure 8. (a) Irradiance plot for the VIS/NIR spectrometer segment show that wavelengths which are 6 nm apart are well resolved. The irradiance plot shows the light power distribution across the area of the detector. The colour bar shows the irradiance value. (b) Vertical cross-section of the irradiance plot shows that the different wavelengths have separated peaks which confirms that they are well resolved.

Similar performance and irradiance analyses have been performed for the SWIR spectrometer segment and equivalent results have been obtained when considering the same specifications for the source. Figure 9 shows the irradiance analysis of the SWIR spectrometer segment. To check the 10 nm resolution, wavelengths with a difference of 10 nm are taken in three regions in its spectral range (lower range at 850 nm, middle range at 1275 nm and upper range at 1285nm). As seen from Figure 9(a), the images of the source at the entry slit for wavelengths separated by 10nm are well distinct for SWIR, showing that the 10 nm resolution has been achieved. Also the vertical cross-section of the irradiance plot in Figure 9(b) confirms that the 10 nm resolution is reached.
Figure 9. (a) Irradiance plot, and (b) vertical cross-section of the irradiance plot for the SWIR segment showing that wavelengths with 10 nm difference are well resolved.

5. CONCLUSION

We have designed a compact two-segment spectrometer which operates in the VIS/NIR and SWIR wavelength range from 400 nm to 1700 nm. The gratings of both segments are blazed to achieve 60% diffraction efficiency in the given wavelength ranges. The spectrometer achieves an SNR of better than 21 dB in the VIS/NIR, and 37 dB in the SWIR range, respectively. Wavelength resolutions of 6 nm for VIS/NIR and 10 nm for SWIR have been obtained theoretically and experimentally. In the future, we will focus on manufacturing the individual optical components, building up the complete one cubic inch spectrometer device and experimentally testing it to validate the simulation results.

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