LEDMET Report: Simulation and correction of stray light in spectrometers

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LEDMET Center for LED Metrology is an innovation konsortium established in January 2014 with focus on problems related to measurements on LED based lighting products. It is a collaboration between Danish National Metrology Institute (DFM), Department of Photonics Engineering (DTU Fotonik), DELTA and Danish Lighting Center (DCL). A large number of lighting companies are participating partners, Louis Poulsen Lighting, Senmatic, ChromaViso, Viso Systems, LightCare, Philips Denmark, Brother, Brother & Sons, North Invent, LEDiBond, LEDProof, Danelec Marine, Martek Marine, Morfoso, Ingemann Components, HAI Horsens, Eclat Digital, and Efsen Engineering. More information and publications can be found on www.ledmet.dk.

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Front page photo shows an incandescent lightbulb seen through a grating, displaying several forms of stray light.
Abstract

In this report, stray light is described as a source of uncertainty in spectrometers and spectroradiometers, and through simulation of various kinds of stray light we show the effects these have on the derived quantities of the spectral measurements. The simulated stray light is then sought corrected by the method developed by Zong et al. at NIST and the derived quantities are then compared to the original data. This report is the deliverable of milestone M1.3 in project Center for LED Metrology (LEDMET).

Sammenfatning

I denne rapport beskrives strejflys (stray light) som en kilde til usikkerhed i spektrometre og spektroradiometer. Gennem simulering af forskellige slags strejflys på spektral data viser vi de effekter som disse kan have på de afledte størrelser fra spektrometermålinger. Det simulerede strejflys søges derefter korrigeret ved metoden udviklet af Zong mf. ved NIST og de afledte størrelser sammenlignes derefter med de originale data. Denne rapport udgør milepæl M1.3 i Center for LED Metrologi (LEDMET).
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1 Introduction

1.1 Scope

This report deals with stray light inside spectrometers. The effect of stray light on measurements is outlined, characterization of stray light is described, and finally it is demonstrated how this characterization can be used for correction of measurement results. The report will serve as an introduction to the field and is not to be considered all-encompassing or authoritative. For more authoritative sources; see the ASTM standard [1] or the coming CIE technical report from technical committee CIE TC 2-51, which is expected to be published in 2018.

In the context of spectrometers, CIE defines stray light as follows [2]:

“in a spectral measurement system: light that reaches the detector, which is at a wavelength other than that which is intended to be measured”

In this context stray light is only the light that is astray after it has passed the input optic of the spectrometer. Stray light from the ambient such as reflection off walls in the laboratory or light from other sources than the device under test is not considered here.

Focus of this report will be on array spectrometers i.e. spectrometers based on grating spectrographs and CCD detector arrays, however the content is not exclusively applicable to this type of instrument.

1.2 Background

Stray light is basically a source of error in spectrometric measurements. The amount of stray light is strongly correlated to the light being measured, so it cannot for instance be detected and characterized without a light source.

Stray light has been a concern for many years, the phenomenon was investigated as early as the 1960ies [3], [4]. The main concern is that the measurement error or measurement uncertainty associated with a given amount of stray light is larger than that which is the needed minimum for a given application. For measurement of broadband integral quantities such as colorimetry and dosimetry, diffuse stray light (see section 2.2.1) is a large issue, due to the large wavelength shift of a part of the radiation, where for instance red/IR stray light will contribute to an erroneous measurement of blue/UV light. For measurement of line spectra the broadening of lines or bandpass (see section 4.3) can be unwanted, due to for instance adjacent lines fusing or the increased uncertainty of the measured wavelength of a given spectral line. Stray light is also a concern in other fields of such as absorbance spectroscopy [5].

A form of stray light that is well known is the effect in photography popularly known as “lens flare”, which typically manifest itself as bright rays or colored shapes forming around very bright objects. As is the case with spectrometers the effect can in normal use be difficult to detect, but becomes apparent when measuring a singular bright object within a dim environment. Figure 1 illustrates this, showing the sunset appearing in the rearview mirror of a car. Here the stray light appears to be “inside” the car, illustrating that the “rays” and other effects in this camera images is a phenomenon related to the camera and not for instance an atmospheric effect.
Inspired by stray light correction in cameras Zong et al. developed in 2006 a method [6], that seem now to have been all but officially named the “Zong method” in the lighting measurement community. Nevas et al. at PTB has worked extensible with the technique [7]–[10] using an optical parametric oscillator (OPO) tunable laser system (see section 5.1.2) to measure the stray light in spectroradiometers.

2 Stray light

This section deals with the various kinds of stray light.

It is important to note that stray light inside the spectrometer, sometimes referred to as internal stray light, cannot be compensated by a measurement with the test source off, due to the fact that light from the actual measurement is the sole contributor to internal stray light.

2.1 Line spread function

The line spread function \( f_{LSF} \) describes the way in which monochromatic light with wavelength \( \lambda_n \) incident on the detector contributes to signals \( S \) at wavelengths \( \lambda_m \)

\[
f_{LSF}(\lambda_n, \lambda_m) = S(\lambda_m) + \sum_{n=1}^{N} a_{n,m} S(\lambda_n)
\]

where \( N \) is the number of measured wavelengths and \( a_{n,m} \) is the transfer coefficient between wavelength \( \lambda_n \) and \( \lambda_m \). A complete characterization of a spectrometer has to contain all values of \( a_{n,m} \), meaning a \( N \times N \) matrix of values.
An ideal line spread function is a rectangular step function, which has zero response for all wavelengths except on the interval of the relevant pixel, this is illustrated Figure 2. This ideal is however not present in any real spectrometer. For a real device the line spread function will look more similar to for instance Figure 4 illustrating broad band diffuse stray light or Figure 8 illustrating line boarding. A typical line spread function features both diffuse stray light and line broadening. Both the diffusion and broadening can be minimized however it cannot be completely removed.

![Graphs showing ideal line spread function](image)

**Figure 2 – An ideal line spread function shown for a large wavelength range (a) and for a zoom in on the pixel with an exact 1 nm response curve, zero for all values except on the interval of the relevant pixel**

2.2 Types of stray light

This section covers some forms of stray light that can have a large effect on spectral measurements.

2.2.1 Diffuse stray light

Diffuse stray light is light that is diffusely reflected by structures inside the spectrometer housing and consequently hits the detector array at all or many pixels.

2.2.2 Bandpass/line broadening

Due to different effects; such as the width of the spectrometer input slit, the grating structure, defocusing of the light on the detector and diffusion processes on the CCD detector, the signal of a single incoming wavelength is spectrally broadened. For most multipurpose spectrometers this broadening is on the order of 1-5 nm, depending on the quality of the spectrometer. This effect is called the band pass of the spectrometer [11].
2.2.3 Specular stray light
Specular stray light is light that is reflected specularly (directly) inside the spectrometer but to other pixels than the intended pixels. The specularity means that only a few pixels will be affected. Specular stray light can have different behavior:

- Specular stray light that have not passed the grating will give a signal proportional to the total spectral light input for the same pixel independent of the spectral power distribution
- Specular stray light that have been refracted by the grating will give a signal proportional to the input light at a given wavelength and the affected pixels will be wavelength dependent, this can include light reflected multiple times by the grating causing complex stray light signal behavior

2.2.4 Out of range stray light
Out of range stray light is light that enters the detector, having a wavelength that is out of the wavelength range of the spectrometer and gives rise to a signal at some wavelengths which is inside the measurement range wavelength. This is typically infrared (IR) and ultraviolet radiation (UV). Stray light in the IR range is generally a problem since many normally absorbing surfaces (for instance inside the spectrometer housing) are highly reflecting in the IR range. Spectral measurements of daylight is particularly vulnerable to out of range stray light, as daylight has both large UV and IR components. Another consideration is that incandescent lamps, which are often used for calibration has a large component of IR radiation. One particular problem with out of range stray light is that it is generally very difficult to numerically correct for, since there no numerical values available for the signal at the out of range wavelengths. Additionally UV radiation gives rise to fluorescence in many materials, which can be a source of stray light, both external and internal.

Out of range stray light is not considered in this report.

2.2.5 Other stray light effects
Other important effects that have been outside the scope of this report are:

- Higher order diffraction (An fundamental effect of diffraction that produces a false signal at the double, triple etc. wavelength)
- Double diffraction (Light hitting the grating several times producing traces across the LSF that are difficult to predict)
- Grating defects (A section of the grating sends light to towards a different wavelength than intended)

These subject will be dealt with in the Technical Reports of CIE TC 2-51 and CIE TC 2-80.

3 Stray light correction
This report will only deal with the stray light correction method presented by Zong et al.[6] due to the simplicity and prevalence of the method.
3.1 Correction calculation

The detailed arguments for the calculation can be found in the paper by Zong et al. [6], so it will only be outlined here.

The line spread functions are used as columns to form a matrix $D$ which is in turn used to find the matrix $A$

$$E_{stray}(\lambda) = E_{in}(\lambda) \ (I - D) = E_{in}(\lambda) \ A,$$

(2)

where $E_{stray}(\lambda)$ is the signal including stray light, $E_{in}$ is the incoming light and $I$ is the identity matrix.

The correction is applied by the following equation

$$E_{in}(\lambda) = A^{-1}E_{stray}(\lambda),$$

(3)

where $A^{-1}$ is the inverted matrix of $A$.

It is worth noting that the Zong paper [6] do not consider the absolute magnitude of the spectral power distribution.

3.2 Interpolating the line spread function

The mathematical functions involved in calculating the correction can be based on standard matrix library's such as the ones found in matlab, excel or Python. Except the step where the $D$ matrix has to be interpolated along diagonal lines and not nearest neighbor or similar standard interpretation techniques. This computational step, although trivial to explain can be expected to take some effort when implementing programmatically due to the non-standard aspects of the problem. Figure 3 shows a conceptual diagram of the lines along which interpretation has to be made. Figure 3 also indicates how the correction matrix is jagged in the low and high part of the measured wavelength range. This issue will increase if few static laser lines are available for the stray light characterization. Furthermore the issue of multiple refracted stray light that does not change diagonally with wavelength (such as higher order refraction) becomes an issue when using this method.
Figure 3 – Conceptual drawing of the interpolation method on a small data set, a spectrometer with 25 pixels and 5 probe wavelengths.

4 Simulation of stray light

Spectrometers are found in many form factors, optical configurations and price ranges from small devices that can be detached to a smart phone to high end laboratory devices costing thousands of euros. Furthermore, many spectrometer devices exhibit complex unique behavior, with the line spread function acting as a kind of fingerprint for the device. So to avoid focusing on a special range of spectrometers this report is based on simulation results, to keep the results general enough to be useful in more situations.

4.1 Simulation method of diffuse stray light

Diffuse stray light can be simulated in a simple way by taking the signal at every wavelength and let it contribute to every other wavelength, using the following equation

\[ E_{\text{sim}}(\lambda) = (I + A_{\text{stray,n,m}})E_{\text{ref}}(\lambda) \]

where \( E_{\text{ref}}(\lambda) \) is the spectral irradiance of the source and \( E_{\text{sim}}(\lambda) \) is the simulated result including stray light, \( I \) is the identity matrix and \( A_{\text{stray,n,m}} \) is a matrix where every entry is the correspondence between one input wavelength \( \lambda_n \) and one measured wavelength \( \lambda_m \). For values \( n = m \) \( A_{\text{stray,n,m}} \) is negative to account for the loss from transfer to other wavelength. The entries in \( A_{\text{stray,n,m}} \) used for this simulation are random numbers in a square distribution, with a mean value given by the stray light level. Figure 4 shows the simulated line spread function for diffuse stray light from a 500 nm monochromatic line.
Other simulated line spread function could of cause be used, but here we have adopted a simple flat noisy profile to again keep the simulation simple and general.

4.2 Diffuse stray light simulation results

The simulation and correction method was implemented in MATLAB at DTU Fotonik and the following results are generated using that software. Figure 5 shows the application of a line spread function constructed using the method described in section 4.1, the example shows the incoming wavelength of an LED and the resulting measurement for three different stray light levels. These show clearly how optical power is transferred from the central wavelengths of the input LED to the surrounding wavelengths. This effect will propagate to quantities derived from the measured values, such as luminous flux, correlated color temperature etc. Figure 6 shows how the correlated color temperature deviates from the reference value due to diffuse stray light. Figure 7 shows the variation in luminous as a function of the stray light level. Figure 6 and Figure 7 also show the corrected values of the derived quantities, to show that significant gains can be made in the precision of the measurement by applying the correction.
Figure 5 – Spectral power distributions of an LED spectrum with different diffuse stray light level, in a linear (a) and a logarithmic plot (b)

Figure 6 – Simulated variation in calculated CCT for a white LED as a function of the level of diffuse stray light
Figure 7 – Contribution from stray light on measurement of luminous flux

It is seen from the figures in this section that stray light correction of diffuse light can potentially reduce the error by up to several orders of magnitude.

The “kinks” in the result curves are likely resulting from the random component of the simulation which would be averaged out by increasing the number of calculations.

In section 4.1 the simulation of diffuse stray light is done with a constant stray light level across the wavelength spectrum, which means the off-diagonal element of $A_{\text{stray,n,m}}$ are essentially similar apart from the noise. However, this is rarely the case for real spectrometers. In many cases, the stray light level is wavelength dependent.

### 4.3 Simulated line broadening/band pass

The band pass can be estimated by measuring the spectrum of a normal laser pointer, which typically has a wavelength much smaller than 1 nm. Figure 8 shows the measured spectrum of a laser line using a hand held spectrometer. Here the line is broadened to a full width half maximum (FWHM) of 6.3 nm. To some extent this broadening can be corrected using the Zong method [6], as seen in Figure 9. Here an LED spectrum has been “broadened” by a normal distribution centered on the incoming wavelength and with a FWHM of 16 nm. This spectrum is then corrected using the Zong method, using a similar line spread function. Figure 10 shows the effect of bandpass and bandpass correction from 1-16 nm. Here it is seen that the correction has a more limited application when approaching smaller values of bandpass. It is possible that the clear minimum in the error of the corrected values stems from fact that here the value of the bandpass in the simulation and the band pass of the instrument supplying the test SPD overlaps – and correcting for a lower band pass actually introduces a larger error. For the error and correction of the correlated color temperature seen in Figure 11
**Figure 8** – Line broadening of a laser line, showing the FWHM of the line

**Figure 9** – Spectral broadening (exaggerated to 16 nm), showing the input (reference) spectrum, the broadened signal and the corrected spectrum in linear a) and logarithmic b) plots.
5 Determination of the line spread function

There exists several ways to estimate the line spread function, with varying accuracy and precision. The principle is to provide a number of narrow band light sources and record the full measured spectrum. The narrower, more powerful, and numerous the light sources the better the characterization. In this section a range of methods are presented.
5.1 Single laser lines

Single laser lines (such as laser pointers) can be obtained cheaply, and be used to get an indication of the line spread function. Sources such as: HeNe lasers (632 nm), green laser diodes (532 nm), blue lasers (473 nm, 405 nm), can be used. However, a correct correction will require more probe wavelengths. The 632 nm HeNe laser has been selected for use to calculate the stray light index of spectrometers known as f_{32}, as defined by the CIE TC2-51[12], in the up-coming technical report. Laser lines have the advantages of being extremely narrow band and with no emitted outside that band. However, obtaining many laser lines can be difficult so interpolation becomes important.

5.1.1 Monochromator

A monochromator with a bright and broad band light source can be used to estimate out of band stray light over a range of wavelengths. This technique has the advantage of being relatively simple to implement with normal components from an optics laboratory. However it lacks the narrow bandwidth to study the size of the band pass for most spectrometers. Furthermore it has a relatively low light output which can be a problem if the spectrometer has a low signal to noise ratio. DTU Fotonik have published a paper on a simplified way to acquire the line spread function using a monochromator and a broad band light source [13].

5.1.2 Tunable laser

The most exact determination of the line spread function requires a tunable laser setup with high stable power output over the wavelength measurement range, and in some cases even larger range. The price for such a setup is normally on the order of 1-2 M€. An example of such a setup is the one at PTB in Germany [8] seen in Figure 12. The cost of a tunable laser system or similar light source will be prohibitive for many applications.

![Figure 12 – The tunable laser setup at PTB, Germany as of November 2015](image)

5.1.3 Filter based approach

To estimate the stray light contribution from a certain source (for instance an LED) in a certain wavelength range a cut-off filter can be applied. This removes all incoming light above or below a given wavelength and any excess signal detected in this range will be related to the stray light. By applying a high quality high or low pass filter in front of the detector during a measurement of a typical light source
the error from stray light can be estimated from the amount of signal that can be observed in the spectral region covered by the filter. This has the advantage of being cheap and simple but the results are specific to the source used.

6 Discussion

6.1 Commercial development

OSRAM has reported on the practical implementation of stray light correction in their LED production [14]. Here the technique was use to lower the uncertainty of the colorimetric properties of single LED packages, which in turn can be used to reduce the binning size within the LED production, which again can increase the value of the final lighting products, due to more consistent colors.

Instrument manufacture Gamma scientific has provided stray light correction for their spectroradiometers for a number of years [15]. Similarly has Instrument Systems recently begun to offer stray light correction for their high end spectrometers and monochromators [16].

One concern in the community about stray light correction is that the full determination and calculation of the associated uncertainty of the correction is a rather large undertaking, due to the fact that the correlations between all elements in the correction matrix has to be considered. And this set of numbers is of the order of $N^3$ where $N$ is the number of pixels, amounting to hundreds of millions numbers for each individual spectrometer.

There are a number of patents pertaining to stray light, both older [17],[18] and newer [19] that might be of interest in respect to different commercial applications.

6.2 CIE work

The technical committee CIE TC2-51 [12] is working on a document with extensive details on stray light in spectrometers, as well as other aspects relating to calibration and application. The work is expected to be published as a technical report in 2016 or 2017 at the latest. DTU Fotonik has contributed to some sections in the document, however it is expected to be very extensive and cover both stray light as well as other aspects of spectrometers. Furthermore the technical committee CIE TC2-80, is engaged in making guidance for spectroradiometry, describing the effects and uncertainties of many experimental aspects, including stray light, this technical report will likely be published in 2018.

7 Conclusion

Stay light in spectrometers can be a cause of significant errors, as seen in the presented simulations. Estimating the effect can be a simple task while full accurate correction can be very large undertaking. The simulation methods presented in this report can be used to estimate the error associated with a given level of stray light. The calculation of the derived quantities such as CCT or luminous flux can easily be applied to other quantities such as colorimetric values or circadian stimulus.
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