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INTELLIGENT PHOTONIC MEASUREMENT FOR SPECTROPHOTOMETERS

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Abstract – Experimental results of intelligent adaptive detection made with spectral sensors are presented.
Firstly for a commercial detector array spectrometer the single entrance slit is replaced by a slit array. Differently patterned one-dimensional arrays are used. There are switched and fixed versions of arrays. An improvement of the detected signal and the signal-to-noise-ratio by the factor 10 has been achieved.
Secondly the measured noisy signal is compared with known expected signals. Weak signals can be detected with an high probability and thus an increased sensitivity.

Keywords: Intelligent measurement, intelligent optical instumentation, spectroscopic measurement

1. INTRODUCTION

A typical application for spectrometric measurements is the quantitative analysis of one or a few known chemical components, which is called monitoring. It is advantageous to use as much of the available light as possible. In contrast to this in spectrometers with a single entrance slit normally only a small fraction of the available light is used, fig. 1 [1 … 3]. This fraction may be increased by widening the slit, but this degrades the spectral resolution and can prevent the spectrometer system from fulfilling its task of detecting and monitoring of spectra which carry important information in high definition details. However, since in monitoring applications only certain specific signal shapes have to be detected by the spectrometer, there will be ways to increase the throughput without loosing but improving the sensitivity to the important detail information by using patterns of small slits.

2. SLIT ARRAYS IN SPECTROMETERS FOR OPTICAL MONITORING

To increase the throughput of a spectrometer while keeping the numerical aperture constant, one has to increase the area of the slit aperture. Since the spectral image at the detector is convolved by the slit shape, increasing the slit width will cause some signal components to vanish as early as the width of the slit becomes in the order of two times the pixel pitch or more. To suppress this effect it would be possible to subdivide the new, wide slit into smaller slits of the initial width and perform Hadamard Multiplexing to determine the spectral image generated by each of the small slits. Similar arrangements are used for measuring spectra of multiple different sources [4] or spectra which have a higher resolution than those produced by a single slit [5]. They are shown in figure 2. The difference here is, that all slits essentially produce the same spectrum as a single slit, i.e. the image of a single slit is Nyquist sampled and all slits are

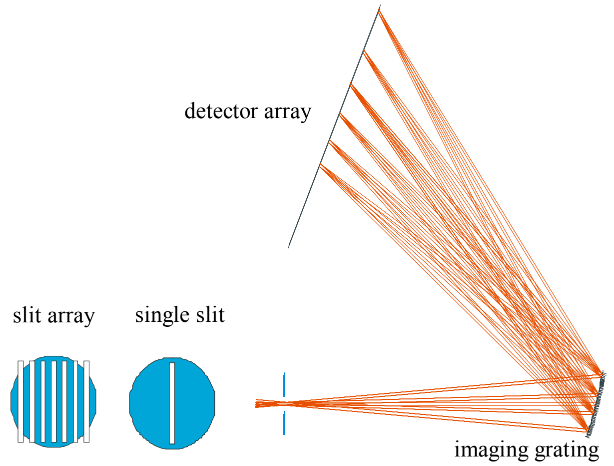

Fig. 1. Detector array spectrometer with an imaging grating, a commercial single entrance slit and a slit array[1, 2] for intelligent sensing; the circle is the illuminated entrance area

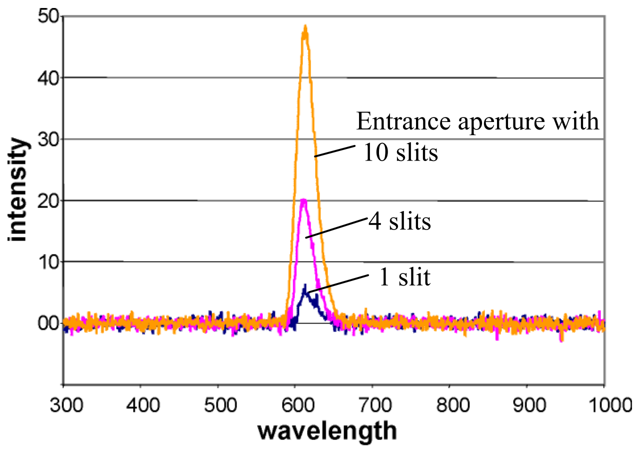

Fig. 5. Signal enhancement by a linear slit array, spectrum with two filters measured with a linear slit-array with 1, 4, 10 slits, spectrometer S10 of Analytik Jena company, the signal is increased compared to a fixed detector noise.

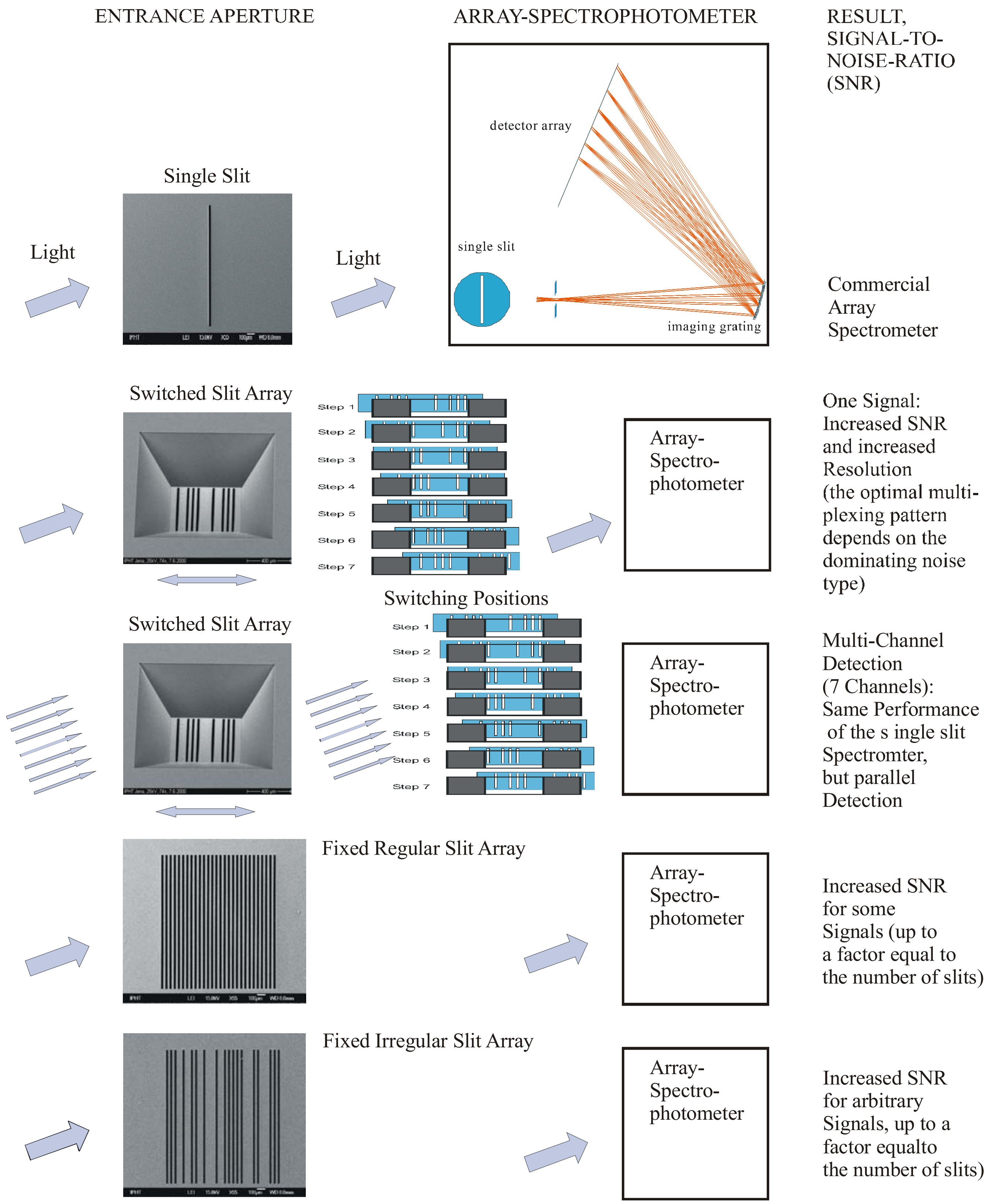

Fig. 2: Entrance apertures [6 … 8] for photonic measurements for spectrometers, the principal arrangement of a commercialspectral sensor, the possibilies of the entrance apertures as a spatial light modulator with switching for multiplexing (selected multiplexing patternin dependence on noise type) and for multichannel signal detection, entrance slit array [6, 7]. for enhanced detection sensitivity of a set of selected signals (monitoring) and irregular slit array for increased (but limited), sensitivity without any restriction to the signals, the entrance aperture chisp are prepared by micromachining technology (REM-picture) with 28 and 18 single slits (width of each slit 25 µm)

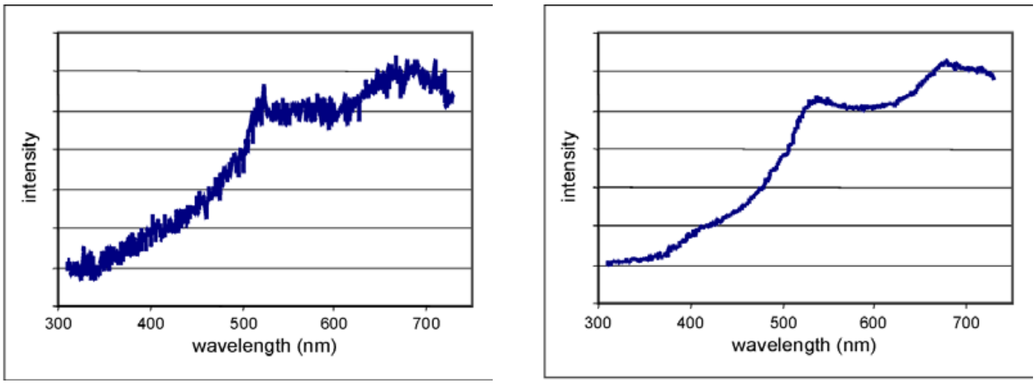

Fig. 3: Increase of SNR of one signal by multiplexing: Spectrum (signal over wavelenth) of a Halogen-lamp detected with a MCS spectral sensor made by the ZEISS company, with a commercial single slit entrance (left) and with a slit positioning system with 11 slits processed in HADAMARD-mode (right). The signal-to-noise-ratio is improved by the factor 1.67±0.3. The theoretical value is 1.81 (in the case of 11 slits). The experimental set-up and the overall measurement time (1.1 sec) was fixed for all measurements.

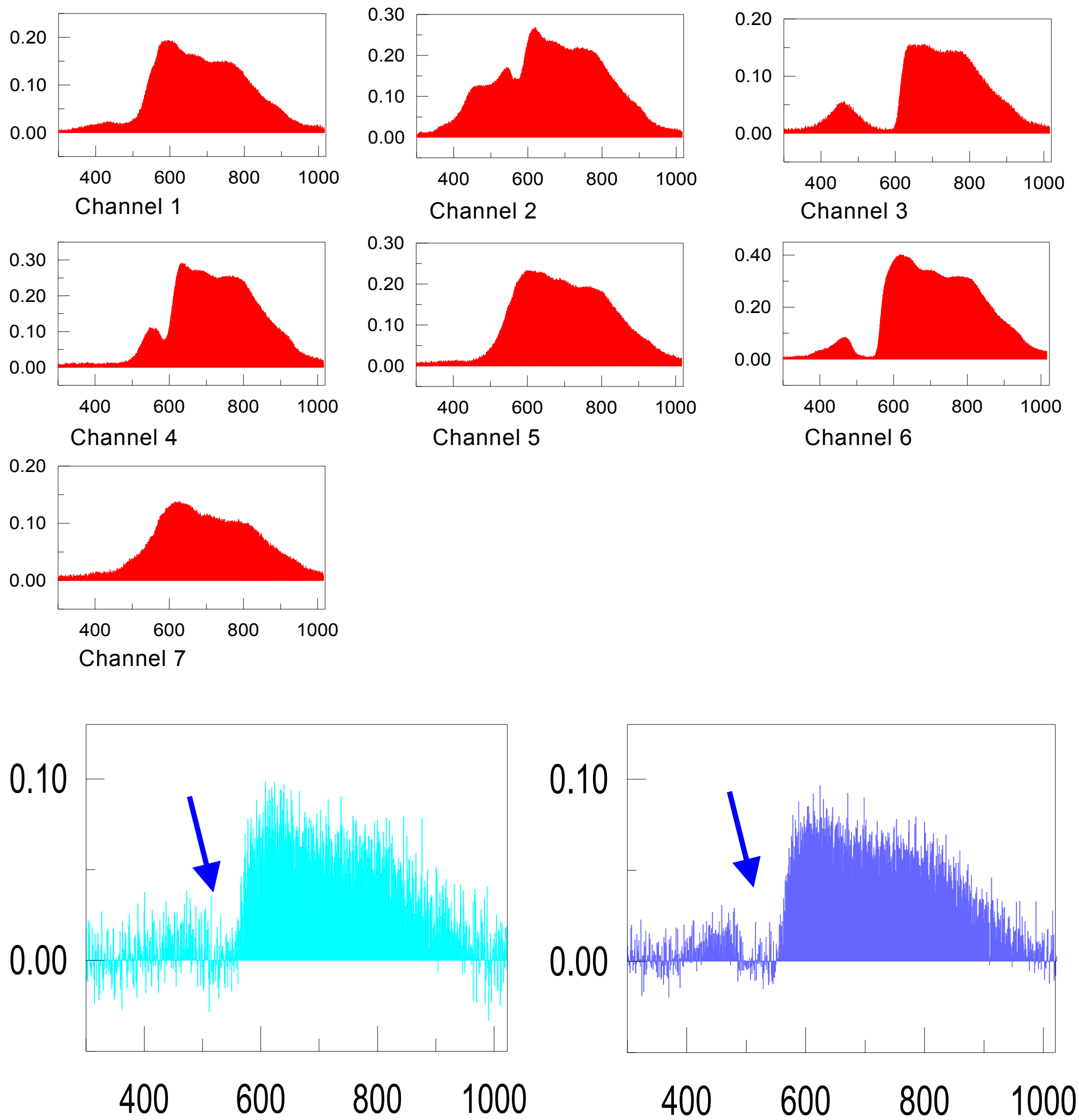

Fig.4: Increase of SNR for multi-channel detection by multiplexing: Spectrum (signal over wavelength in nm) of 7 different dyes (top) and single spectrum of one dye, measured by scanning (bottom left) and by Hadamard-multiplexing (bottom right) with a MCS spectral sensor made by the ZEISS company, the SNR increase in case of 7-channel multiplexing by the factor 1.5

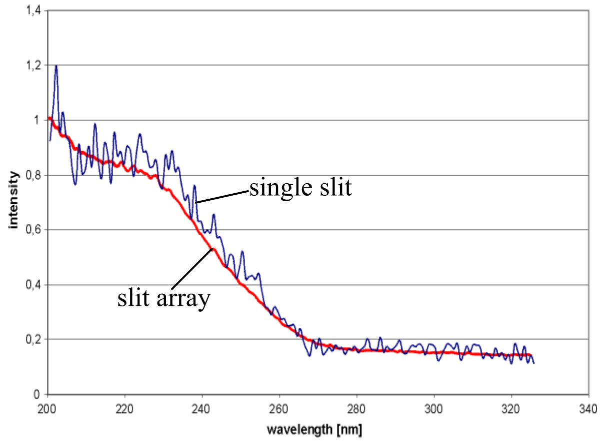

Fig. 6. Spectral detection of DNS with a common single slit spectrometer and with the same instrument, but with a linear slit array with 10 slits. The signal-to-noise-ratio is increased, so the detectable concentration and/or the sample volume can be further reduced.

illuminated by the same source. Compared to a scan, the signal to noise ratio (SNR) of a Hadamard switching [9, 10]. regime would be improved by (N+1)/(2 √N), where N is the number of slits or measurement steps, respectively. If the detector is limited by dark current noise or other noise increasing with the square root of the integration time, the SNR of N averaged measurements of the scanning regime would be equal to the SNR for a single, fixed slit, keeping the overall measurement time constant. Thus, by going to the Hadamard regime, the full Hadamard gain would be achieved.

However, for a read noise limited detector, i.e. one which shows a time-independent noise level, subdividing the overall measurement time into N measurement steps would result in a disadvantage of 1/√N after averaging all measurements of a scan. Going to the Hadamard regime, we would still be left with a disadvantage of approximately 0.5. The Hadamard switching of the slit array is needed to recover the spectral image as it would be produced by a single, small slit or, in other words, to recover all signal components of the spectrum. Experimental results are given in fig. 3 and 4.

Within its specifications the dispersive spectrometer with a single slit, a single scanning slit or a Hadamard switching array (figures 2, 3 and 4) can detect all spectral shapes with the same efficiency. As pointed out above, the purpose of a monitoring measurement is restricted to the detection of signals which are already known or to the determination of a few signal parameters of otherwise known signals. This task is essentially different from the task of simply obtaining a spectral image and normally only a few of the signal components of the spectral image are really involved. Thus we can effort loosing the unimportant signal components while improving the important signal components at their expense. Which signal components are improved and which are suppressed is determined by the slit pattern which we can choose arbitrarily. The monitoring task is then accomplished by measuring a spectral image generated by a certain slit pattern and determining the searched signal probabilities or parameter values directly in the measured spectral image rather than in a deconvolved one. Signal parameters for which sensitivity is improved could - for example - be amplitudes, line widths or the ratio of two line heights.

Effectively, by using slit arrays instead of a single slit the throughput of the spectrometer in terms of transmitted energy can be increased. The effect is shown in fig. 5. A simple example in life sciences with a linear regular slit array consisting of 10 slits is given in fig. 6. An example of an irregular slit array with 18 slits is given at the bottom of fig. 2.

3. SEARCH FOR KNOWN SIGNALS AND MASK DESIGN

In the simplest case the monitoring task is that of comparing the measured signal **g** to some discrete possibilities for an underlying signal **f**, the signal hypotheses $\mathbf{q}^k$. For instance this could be the possibilities $\mathbf{q}^1$="spectrum of substance 1", $\mathbf{q}^2$="spectrum of substance 2" and $\mathbf{q}^0$="no signal". Depending on the measured signal **g**, each possibility has a probability which is given by

$$p(\vec{f}=\vec{q}^k \mid \vec{g}) = \frac{p(\vec{q}^k)}{p(\vec{g})} p(\vec{g} \mid \vec{f}=\vec{q}^k)$$

where $p(\mathbf{q}^k)$ is the a-priori probability of the k-th signal hypothesis and $p(\mathbf{g}|\mathbf{f}=\mathbf{q}^k)$ is the signal production probability or likelihood [13], i.e. the probability density that the measured signal is produced by degrading the supposed original signal. For Gaussian noise with no additional disturbances the likelihood is given by

$$p(\vec{g} \mid \vec{f}=\vec{q}^k) = \left(\frac{1}{\sigma\sqrt{2\pi}}\right)^{N_p} \exp\left(-\frac{1}{2\sigma^2}\sum_j^{N_p}\left(q_j^k - g_j\right)^2\right),$$

where N_p is the number of sampling points and σ is the noise level. In the given formulas it is already supposed, that the measured signal **g** can only be caused by an underlying signal which is one of the signal hypotheses. This restriction leads to an increased sensitivity, as shown in fig. 7. If other types of noise or additional perturbations such as stray light are considered, the above formula for the likelihood will change, but the principle of restriction to certain signals remains unchanged. The faster the detection probability goes towards 1 (0) for the true (wrong) signal with increasing signal-to-noise ratio, the higher is the discrimination capability of the spectrometer for the given hypotheses. The sensitivity of the spectrometer is optimized by using a slit pattern which changes f and $\{q^k\}$ in a way that the discrimination capability is maximized. For the example of pure gaussian noise replacing the single slit by a slit pattern would change the likelihood to

$$p(\vec{g} \mid \vec{f}=\vec{q}^k, \vec{h}) = \left(\frac{1}{\sigma\sqrt{2\pi}}\right)^{N_p} \exp\left(-\frac{1}{2\sigma^2}\sum_j^{N_p}\left([\vec{h} * \vec{q}^k]_j - g_j\right)^2\right),$$

where **h** is a response function imposed by the slit shape and "*" denotes a convolution.

As a special case it is possible to construct masks which give a certain gain for every signal shape. Assuming the

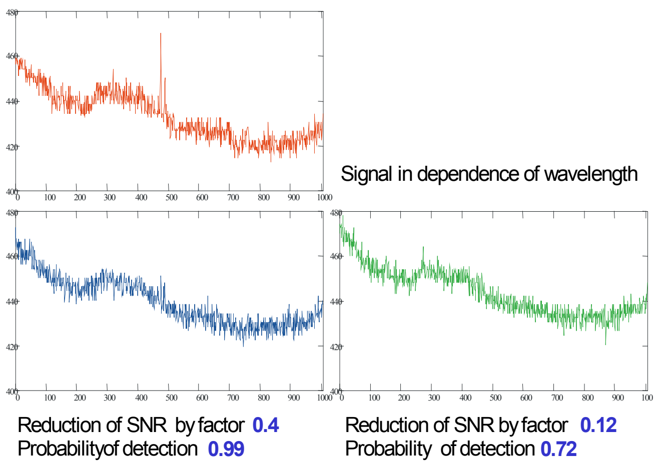

Fig. 7. Search for known signals, a weak emission line of a Na vapor lamp (top). Experiments with reduction of the amplitude of the emission line (bottom) the line is not (well) visible but by search for the known line it is detectable with 99 % and 72 %, respectively. The sensitivity is increased by intelligent signal processing.

optical properties of the spectrometer are completely known, such masks would even allow for the reconstruction of a single slit spectrum from the measured convolved spectrum without a sensitivity loss. Such a mask is shown at the bottom of figure 2.

4. CONCLUSIONS AND OUTLOOK

4.1. Conclusions

A modern development for highly sensitive photonic measurements is discussed at the example of array spectral sensors. New entrance aperture architectures are used. A MEMS version, transmissive slit masks, are discussed.
The aim is to increase the sensitivity of the sensor by enhancement of the signal and the signal-to noise ratio (SNR) - and not by increase of the detectivity of the detector itself.
By using selected slit patterns as entrance arrays the sensitivity can be increased typically by up to one order. For a search of known signals or extraction of a few signal parameters in an otherwise known signal (monitoring) fixed slit masks can be used. Linear entrance slit arrays with up to 28 slits were prepared. The increase of SNR for selected signals will be up to the factor 28. An increase of SNR of the factor 10 has been achieved in experiments with 10 slits.
The entrance aperture architecture can be combined with intelligent signal processing of selected photonic measurements. The simulation of the probabilities and experimental results applied for photonic measurements will be published elsewhere.
In analogy the results can be applied to other measurement arrangements.

4.2. Outlook

If there is a rather large number of signal hypotheses, a single slit pattern will normally not give the optimal discrimination capability. Instead it may be better to do a first measurement with a certain mask pattern which allows a reduction of the eligible signal hypotheses and, depending on this, choose a second mask pattern which gives the best discrimination capabilities for the remaining hypotheses or which allows the most sensitive determination of signal parameters of a single remaining hypothesis. This adaptive process can be carried out autonomously by the spectrometer control which, as a result, shows a simple kind of intelligent behaviour. On the hardware side this will require either arrays of freely switchable slits, such as micro mirror or micro shutter arrays or a means to select precoded slit patterns by moving or exchanging the whole slit mask.

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