Application-Specific Optimization of Near-Infrared Spectral Sensors

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Spectral sensing is attracting increasing interest for the analysis of materials throughout a wide variety of applications. The use of light provides a fast and non-destructive way to investigate the chemical composition of materials. We have recently reported a fully-integrated, robust and low-cost near-infrared (900-1700nm) spectral sensor consisting of resonant-cavity-enhanced photodetectors. Here we report an approach to optimize its spectral response for specific applications. We use the transfer-matrix method to simulate the response of the sensor and predict the performance for known reflection or transmission spectra from a specific sensing problem. A particle swarm optimization is used to find a design providing optimized sensing accuracy, which can be a non-trivial combination of resonant wavelengths.

Introduction

There is substantial interest in spectral sensing for the analysis of materials in a wide variety of applications, as it allows for a fast and non-destructive method to measure the chemical composition of materials. Specifically, near-infrared (NIR) spectral sensing has seen increasing progress in past years. The NIR region contains first and second overtones of C-H, OH and N-H molecular bonds, as well as combinations of these vibrational modes. Due to the overlapping nature of these absorption bands, the features in NIR spectra are often broad and hard to interpret directly [1] and chemometric methods are used to build predictive models [2].

For most in-field and in-line applications, small, portable and affordable sensors are needed, which has motivated research in miniaturization and wafer-scale fabrication. There are a variety of ways to miniaturize spectral sensors [3]. While spectrometers based on waveguide circuits are compact and mass-manufacturable, their limited spectral range and very small input étendue (and thereby the impossibility to efficiently couple incoherent light from a large area) makes them unsuitable for most in-line and portable sensing applications. We have previously demonstrated an approach to spectral sensing based on an array of 16 resonant-cavity enhanced (RCE) detectors as a compact, robust and low-cost solution [4]. Fig. 1a provides an optical image of such a spectral sensor. By varying the thickness of a tuning layer inside the cavity, the resonance of each detector (pixel) can be shifted to different wavelengths. The spectral response of the multipixel array (Fig. 1b) displays peaks with full-width half-maximum FWHM≈60nm and high peak responsivity (R=0.3A/W). While the sensor does not measure the full incident spectrum, the generated photocurrents allow us to retrieve information from the object [4]. The effectiveness of this approach has recently been demonstrated on a variety of real-life applications using a standard configuration of our sensor [5, 6].

While the present sensor has general applicability, we can ask the question what the best configuration of the sensor is for a given application. Indeed, for a given problem only certain spectral bands carry relevant information and the data from some pixels is not used in the prediction models. Using less and larger pixels with response in the most relevant spectral bands would provide a higher signal-to-noise ratio (SNR) for a given total sensor area. It is therefore attractive to determine the minimum number of pixels required for a given problem and exploit the higher SNR to improve sensing performance. A similar optimization of sensor spectra has been reported previously in the context of filter arrays [7, 8]. Here we report an approach to find the optimal configuration of resonant-cavity detector structures for a specific sensing problem, with variable number of pixels and SNR.

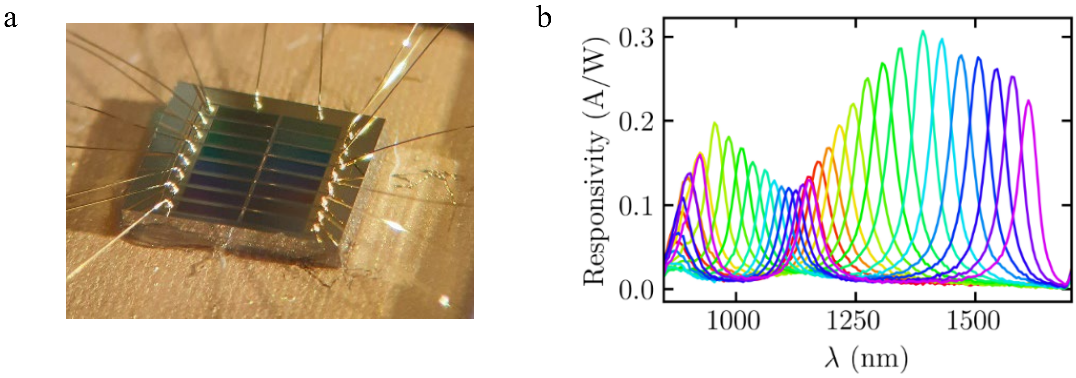

Figure 1 *a) Image of the multipixel array with 16 resonant-cavity enhanced detectors. b) Measured responsivity curves for each of the pixels in the array.*

Methods

A schematic of the optimization procedure is displayed in Fig. 2. In order to demonstrate the approach, a dataset with transmission spectra for varying concentrations of methanol in isopropanol was experimentally acquired. This problem was chosen because of the high reproducibility across multiple experiments. A specific application is characterized by a dataset of transmission spectra from the solution along with calibrated values (the concentration of methanol). The responsivity curves for an arbitrary configuration are calculated using the transfer-matrix method. The resulting expected photocurrents are then determined by multiplying the incident spectra with the responsivity curves. Variable Gaussian noise is added to these photocurrents, to simulate the read-out noise during an actual experiment. A part of the resulting dataset is used to train a model, whereas the rest is used to test how well this model is able to predict the calibrated values from the photocurrents. This results in a value for the ratio of performance to deviation, or RPD, which is the ratio between the standard deviation of the calibrated values and the root-mean-square error of prediction by the model. The RPD is used as the figure of merit (FOM) for the optimization.

The FOM is optimized using a particle swarm optimization (PSO). Here, the thicknesses of the tuning layers are the degrees of freedom. During the optimization the fabrication constraints, such as the range of thicknesses that are feasible to deposit and the combinations that are possible with the layout of available optical lithography masks, are taken into account. Each particle consists of a set of response curves and a resulting calculated RPD. During each iteration the particles move towards a new position based on the best positions within the group, their neighbors and their own memory. When the FOM no longer improves over multiple iterations, the optimization is finished.

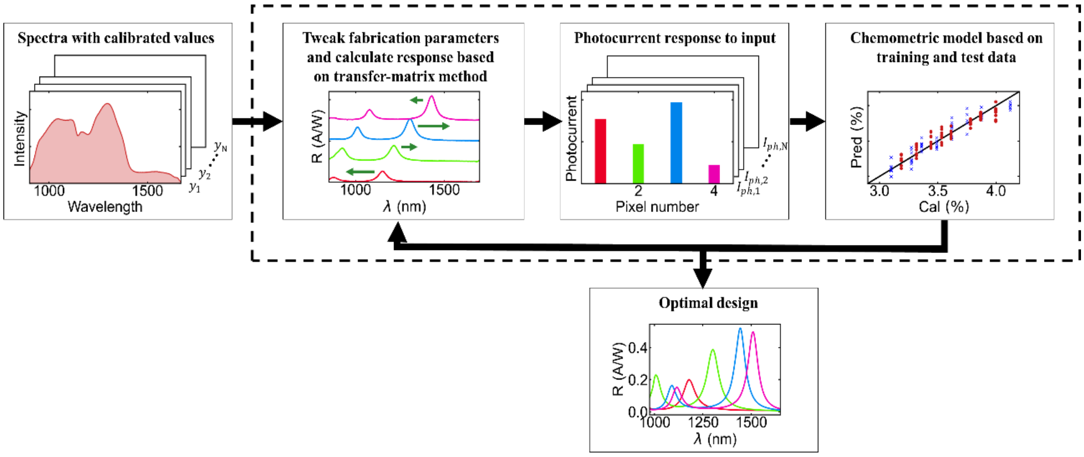

Figure 2 *Schematic of the application specific optimization procedure. The steps in the dashed lines are part of the particle swarm optimization, where each particle is a configuration of the sensor. When the figure of merit has not improved for many iterations anymore, the optimal design is taken from the memory of the particles.*

Results and discussion

Fig. 3 shows the results of the optimization procedure for this problem using a configuration with 4 pixels and a noise corresponding to an SNR of 19000 on average over all pixels. There were 500 particles in the swarm, which are initially distributed evenly over the design space. The RPD at iteration 0 is the best solution among these initial particles (therefore already higher than the average for a random configuration) and can then be seen to increase over 27 iterations (Fig 3a). The FOM shows plateaus and increases at specific steps. This is because the optimal solution does not improve by simply shifting the wavelength continuously. There might be specific wavelength ranges that are of importance and that need to be reached before the FOM improves. Fig 3b shows the final prediction on the dataset, where the calibration data was used to train the model and the test data used to calculate the prediction strength. Fig 3d shows the simulated responsivity curves for the optimal solution. During the optimization the FOM reaches RPD=15.8 and when testing the sensor on data that was not part of the optimization it has an RPD=12.8. This RPD indicates high sensing performance. A tolerance analysis to fabrication errors is shown in Fig 3c. The thicknesses of the optimized design are changed by randomly adding deviations with a normal distribution with standard deviation σ, after which the RPD is calculated again. This is done multiple times for each σ to get an average RPD. For increasing levels of deviation from the design, the RPD can be seen to always be less than the optimum. Sometimes a slight increase can be seen for higher values of σ, this is again due to the effect of specific wavelength ranges that can be of higher importance than others.

The optimal number of pixels heavily depends on the sensing problem and on the noise level of the read-out. If the read-out is not too noisy, increasing the number of pixels generally improves the performance. Also, a larger number of pixels improves the robustness to fabrication errors. For larger noise levels, the trade-off between number of pixels and the resulting decreasing SNR becomes more important and the optimization procedure can add more value. The main advantage of using an optimization procedure, as compared to handpicking the wavelengths, is that it takes all combinations of bands into account, while also including the influence of noise on the read-out.

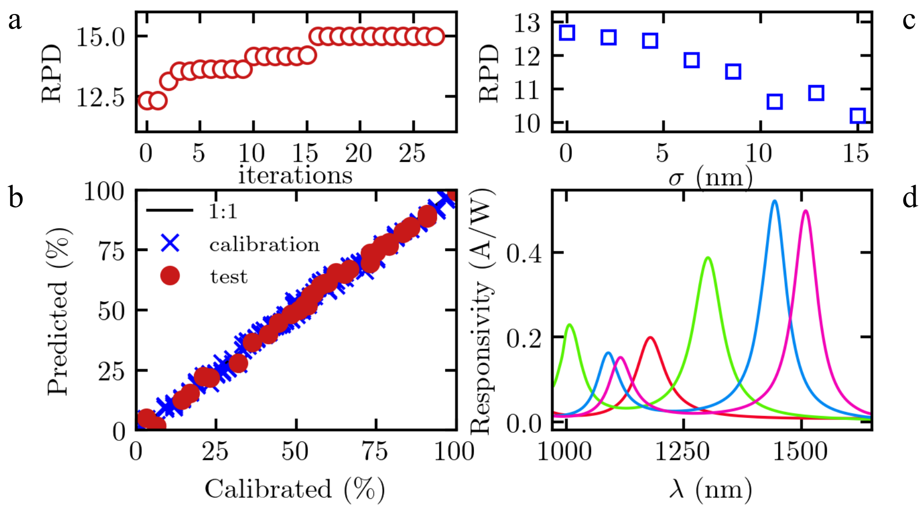

Figure 3 *Results of the particle swarm optimization for sensing the concentration of methanol in isopropanol for a 4 pixel configuration.. a) shows the evolution of the RPD corresponding to the best solutions found in the swarm throughout the iterations of the optimization. b) displays the final predictions strength corresponding to a particle with responsivity curves as shown in d). The tolerance to deviations in fabrication is shown in c), where random deviations are added to the thicknesses of the optimized design with a normal distrubtion with standard deviation* σ.

Conclusion

Miniaturized spectral sensors based on detector arrays are a powerful tool for real-time and in-field analysis of materials. Here, we described an approach to optimize the response of a spectral sensor for a specific application using a pre-calibrated spectral dataset. The resulting design can be a non-trivial combination of resonant wavelengths, taking into account the SNR of the read-out system. The procedure is applied to the case of determining the concentration of methanol in isopropanol and shows the potential for high performance, even using a small number of detectors.

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References

[1] Ozaki, Y. et al. Near-Infrared Spectroscopy. *Springer*; 2021
[2] Pasquini, C. et al. Near infrared spectroscopy: A mature analytical technique with new perspectives – A review. *Analytica Chimica Acta*; 2018
[3] Zongyin, Y. et al. Miniaturization of optical spectrometers. *Science*; 2022
[4] Hakkel K.D. et al. Integrated near-infrared spectral sensing. *Nat Communications*; 2022
[5] Ou F. et al. Handheld NIR Spectral Sensor Module Based on a Fully-Integrated Detector Array. *Sensors*; 2022
[6] Kranenburg R.F. et al. On-site illicit-drug detection with an integrated near-infrared spectral sensor: A proof of concept, *Talanta;* 2022
[7] Soyemi, O. et al. Design and testing of a multivariate optical element: The first demonstration of multivariate optical computing for predictive spectroscopy. *Analytical Chemistry*; 2001
[8] Tan, H. et al. Genetic optimization of mid-infrared filters for a machine learning chemical classifier. *Opt. Express;* 2022