LabVIEW-based Program for Peak Detection and Curve Fitting of Spectral Data for On-chip High-Sensitivity Real-Time Optical Spectroscopic Bio/Gas Sensing Applications

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Abstract: We present a LabVIEW-based spectrum analysis and software package integrated with the on-chip nanophotonic biosensor and demonstrate its use for spectral peak analysis, curve fitting, and background noise subtraction.

1. Introduction

In sensing experiments, the spectroscopic spectral data is generally perturbed due to electronic noise and environmental variations such as temperature, pressure, humidity, and density. The spectral line profile, therefore, experiences a shift in peak location, line broadening, and line overlapping. Consequently, the accurate spectral data analysis of optical-based spectroscopic sensors requires further data analysis techniques. For example, the wavelength/frequency modulation spectroscopy technique utilizes a conventional and useful electronic Lock-in Amplifier to generate higher harmonic signals, enhance sensitivity and specificity, resolve spectral line resolution, and accurately detect peak location. However, the LabVIEW-base software we present here can generate first and second harmonics (1f and 2f) without needing the bulky Lock-in Amplifier. This presented software program will be demonstrated to analyze spectral data resulting from our on-chip biosensors employed for biomedical and environmental applications. It can be used for analyzing any shape of spectral line profiles (for example, Lorentzian, Gaussian, or Voigt).

2. The Method & Methodology

2.1 Bio-Sensing Spectrum

First, our lab-on-a-chip biosensor is built upon the subwavelength grating waveguide-based micro-ring resonator (SWGMR) with high sensitivity and low limit of detection (LOD). SWGMR provides a pathway to manipulate optical properties such as dispersion and refractive index [1] and a platform for biosensing applications needing fast screening and early diagnosis. The SWGMR design structure is shown in Fig 1. The light entering a waveguide bus is coupled into the ring resonator, producing detectable optical signals due to index perturbations. The ring spectral modes resonate at a wavelength($\lambda_{\text{resonance}}$) which is given as: $\lambda_{resonance} = \frac{L}{m} n_{eff}$. The resonance mode spectrum shows sharp dips in the transmission, as shown in Fig. 2. A change in the ring surface's refractive index makes the $\lambda_{\text{resonance}}$ shift ($\Delta\lambda$), and the resonance spectrum can be monitored by scanning wavelength through an optical spectral analyzer (OSA). The size of the $\Delta\lambda$ is proportional to the number of adsorbed analytes. Fig. 1. (b) depicts a microfluidic system that can be integrated with a lab-on-a-chip SWGMR for point-of-care diagnoses, such as COVID-19 detection.

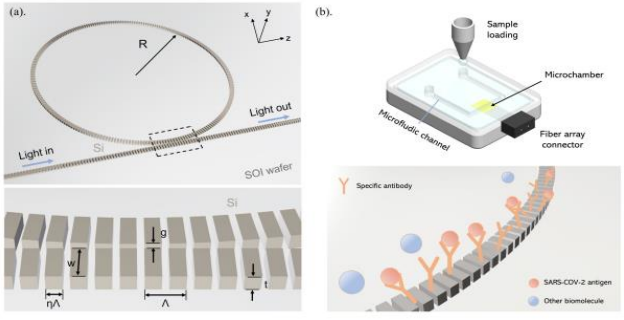

Fig. 1. Schematic of SWGMR biosensor. (a). Device schematic (b). Microfluidic system schematic. [2]

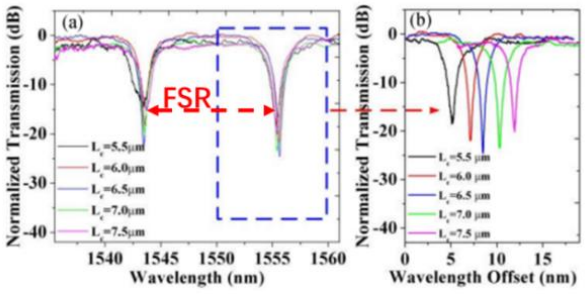

Fig. 2. (a) The transmission spectra of the fabricated five SGMRTRs. (b) Magnified resonance dips in blue dashed rectangular region in (a).[1]

2.2 Data Analysis Algorithm

This section describes the outlines of the dedicated virtual instrument (VI) program developed using LabVIEW software to analyze spectra obtained from the sensors as mentioned above. Fig. 3. illustrates that the algorithm involves several steps and parameters. First, the LabVIEW read raw data of wavelengths and power intensity from OSA. The next step is noise reduction. The Kernel Density Estimation (KDE) method is implemented for data smoothing purposes at this step. Next, the peak window detection algorithm can automatically find the peak window. Next, the peak window detection algorithm can automatically find the peak window. Then, the start and end points are defined from the entire spectrum data range to search for peaks. Fig. 2. (b) depicts the 1st and 2nd derivative processes where the algorithm can define the peak windows by threshold value to identify the range of windows to search for peaks in the spectrum. Last is the curve fitting process, the bio-sensing spectrum is based on the SWGMR structure, and the power transfer(T_{ap}) function of the through-port is as follows[3]:

$$T_{ap}(\phi_{rt}) = \frac{T_{ap,min} + F\,sin^2(\frac{\phi_{rt}}{2})}{1 + F\,sin^2(\frac{\phi_{rt}}{2})} \quad (1)$$

We assume this $\sin^2$ (x) function and 2nd order polynomial function are similar when the roundtrip phase detune (ϕ_{rt}) is relatively small. The General Polynomial Fit.vi can be implemented to generate a nearly fitting formula, and the $\lambda_{resonance}$ can be extracted by mathematical calculation. Furthermore, the Q value and the Free Space Range (FSR) can be determined to estimate the fabricated quality of each bio-sensing chip.

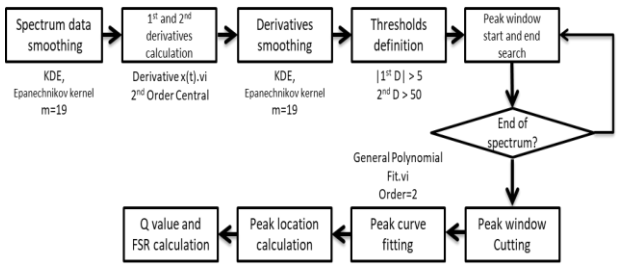

Fig. 3. Flowchart of the peak minimum location determination algorithm.

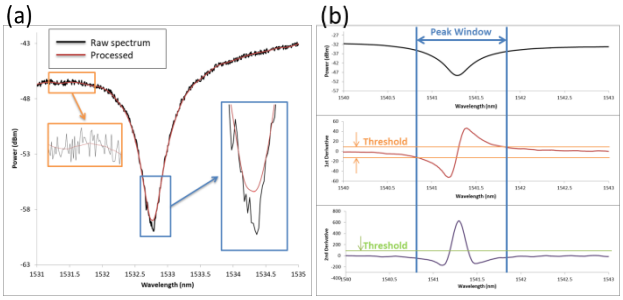

Fig. 4. (a) The high noise real bio sensing spectrum. (b) Raw spectrum, first and second derivatives of real bio sensing sample.

3. Results and Discussions

We use real bio-sensing spectrum data sets to evaluate the performance of the data analysis algorithm. Fig. 5. illustrates the noise level of real-time $\Delta\lambda$ tracking results down to a low degree when the curve fitting algorithm is implemented. Table 1 shows that the data analysis algorithm can reduce the RSD from 83.2% to 9.7% and notably decrease LOD from 38.38 pm to 4.46 pm. Fig. 6. demonstrates real-time $\lambda_{resonance}$ identification results with the algorithm processed, and this practical experiment data can confirm the stability and reliability of this algorithm.

Table 1. Compare to raw spectrum

Methods	STD (pm)	RSD (%)	LOD (pm)
Raw Spectrum	12.79	83.2	38.38
Processed	1.48	9.7	4.46

*STD = standard deviation
**RSD = relative standard deviation
***LOD = low limit of detection

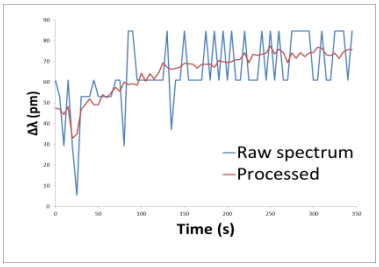

Fig. 5. Real-time $\Delta\lambda$ analysis with algorithm implemented.

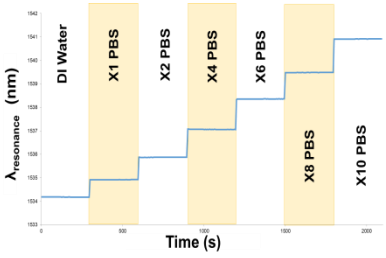

Fig. 6. Real-time biosensing results

4. Conclusions

We propose an efficient and robust peak detection and curve fitting algorithm to analyze bio-sensing spectrums, precisely identify $\lambda_{resonance}$, and track the shift of $\lambda_{resonance}$. By processing this algorithm for real-time biosensing spectrum, we can observe that this algorithm significantly improves the reliability of the results of our bio-sensing systems. Furthermore, the algorithm can improve the quality of analysis of the bio-sensing spectrum and can be used on other types of the spectrum to analyze profiles.

References

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