Micrograting design to retrieve IR spectra in the long wavelength region

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To design microgratings, which can be used for correlation spectroscopy in the 725–1450 cm⁻¹ range, a gradient searching Davidon–Fletcher–Powell (DFP) algorithm was successfully applied to retrieve target spectra of SF₆, ethylene, SO₂, and NH₃. Owing to a unique fit parameter treatment, the DFP algorithm produced stable convergence for the minimization and provided superior matches between the diffraction spectrum and the target spectrum to those provided by the phase retrieval algorithm (PRA) or the extended PRA. In addition, the diffraction efficiencies for the micrograting line profiles obtained from the DFP algorithm were at least an order of magnitude greater than those from the PRA or the extended PRA. We also evaluated the effects of number of line element reduction or the dimensional errors in the line elements on the spectrum shape. The line depth error would not change the main spectral features but increase noise features. However, the line width error affects more sensitively the spectrum shape and the diffraction efficiency.

Keywords: micrograting; phase retrieval algorithm; gradient search; Davidon–Fletcher–Powell algorithm; correlation spectroscopy; IR spectrum

1. Introduction

One of promising products in MEMS technology is the micrograting, which may take over numerous optical components such as conventional gratings with fixed pitch. Unlike conventional gratings, the diffracted light off a micrograting may display a desired spectrum. Such a merit of the micrograting is well recognized in correlation spectroscopy [1–3], in which the presence of a target molecule in a sample mixture can be identified through a cross-correlation between the target spectrum and the sample spectrum. As the micrograting can replace the target spectrum, preparing the target cell in the correlation spectrometer is no longer necessary. Once the micrograting structure is varied by actuators and electronic control, many target spectra can be generated from a single actuated micrograting.

The correlation spectrometer would be most useful when the target spectrum exhibits sharp peaks, as in IR spectra of gas molecules. The first proposal of the micrograting to be used for IR correlation spectroscopy of gas molecules was made over a decade ago by Sinclair et al. [2,3]. In their scheme, the micrograting plane is faced normal to the incident direction of broadband light, and the diffraction off an array of reflecting line elements of the micrograting is detected at a fixed angle θ (Figure 1). The micrograting pattern or the line elements depth profile must be designed to retrieve the spectrum of target gas.

1.1. Phase retrieval algorithm

Sinclair et al. used a phase retrieval algorithm (PRA), which is similar to two-dimensional digital image reconstruction methods [4,5]. Based on the Gerchberg–Saxton algorithm [6], the PRA begins with a randomly generated phase array and a constant reflection amplitude array (usually set to 1) in the micrograting domain. The combined complex array is Fourier transformed to give the amplitude and the phase arrays in the diffraction domain under the Fraunhoffer approximation [7]. The amplitude array is then replaced by the target spectrum amplitude, and the recombined complex array is inversely Fourier transformed into the micrograting domain. The combined complex array is Fourier transformed to give the amplitude and the phase arrays in the diffraction domain under the Fraunhoffer approximation [7]. The amplitude array is then replaced by the target spectrum amplitude, and the recombined complex array is inversely Fourier transformed into the micrograting domain. This process is iterated. In each iteration loop, a unit reflectivity replaces the amplitude array in the micrograting domain and the target spectrum amplitude replaces the amplitude array in the diffraction domain. After hundreds of iteration loops the diffraction spectrum is converged to the target spectrum. The final phase array φᵅ in the micrograting domain is then transformed to the depth array dᵅ of the micrograting line elements according to
where \( M \) is the number of line elements and \( \lambda_0 \) is an arbitrary wavelength in the spectrum.

Although the PRA appeared to retrieve qualitatively the spectra of a few gas molecules such as HF in the 3600–4300 cm\(^{-1}\) range [2,3], its inherent drawbacks need be mentioned. Firstly, since the PRA relies on the iterative Fourier transform, the number of sampling points in the target spectrum is limited to the number of line elements \( M \), which is determined by the spectral region of interest and the overall micrograting size. In practice, Sinclair et al. note that only \( M/4 \) points must be sampled in the spectral region of interest [2].

Secondly, while the depth profile \( \{d_m\} \) produces the wavelength dependent phase profile \( \{\phi_m\} \), the relation in Equation (1) is independent of wavelength and the synthetic diffraction spectrum deviates from the desired spectrum as the wavelength deviates from \( \lambda_0 \). Thirdly, as the PRA is not truly a minimization process based on error reduction, it is likely to converge into a local minimum.

The lack of sampling points in the target spectrum can be overcome in an extended PRA [8]. In this method, the target spectrum is oversampled to \( 2M \) or \( 4M \). The increased extra line elements are positioned outside the usable area of the micrograting with zero reflectivity while only \( M \) line elements are positioned inside the usable area with a unit reflectivity.

### 1.2. Gradient search method

The drawback of the PRA necessitates an optimization method based on error reduction. In such a method, the difference between the target spectrum and the diffraction spectrum is to be minimized with the depths of line elements as the fit parameters.

Working in the Fraunhofer approximation [7], the diffracted field at \( \theta \) is described by

\[
U(\lambda) = \frac{C}{\lambda} \int_{-\infty}^{\infty} U'(x, \lambda) \exp \left(-i \frac{2\pi \lambda \sin \theta}{\lambda} \right) dx,
\]

where \( x \) is directed along the micrograting plane (Figure 1) and \( C \) is a constant. \( U'(x, \lambda) \) is the near field just leaving the micrograting and can be expressed as the sum of contributions of all line elements by

\[
U'(x, \lambda) = \sum_{m=1}^{M} \exp \left(-i \frac{4\pi d_m}{\lambda} \right) \text{rect} \left( \frac{x - m\Delta + \Delta/2}{\Delta} \right),
\]

where \( \Delta \) is the width of the line elements and \text{rect} represents the rectangular function. The depths of the line elements \( d_m \) must have values between 0 and \( \lambda_{\text{max}}/2 \), where \( \lambda_{\text{max}} \) is the maximum wavelength in the spectral region of interest.

Zhou et al. [9] have shown that when the spectrum is sampled at wavenumbers \( \tilde{\nu}_n (n = 1, 2, \ldots, N) \), \( U(\lambda) \) in Equation (2) is reduced to \( U_n \) in

\[
U_n = \exp(i\tilde{\nu}_n \Delta \sin \theta) \sum_{m=1}^{M} G_{mn} \exp(-i4\pi d_m \tilde{\nu}_n),
\]

where

\[
G_{mn} = C \tilde{\nu}_n \Delta \text{sinc}(\tilde{\nu}_n \Delta \sin \theta) \exp(-i2\pi m \Delta \tilde{\nu}_n \Delta \sin \theta).
\]

The error \( Err \) between the target spectrum intensity \( I'_n \) and the calculated diffraction spectrum intensity \( I_n \) is defined as

\[
Err = \frac{1}{N} \sum_{n=1}^{N} \left( I'_n - \gamma I_n \right)^2;
\]

where \( I_n = |U_n|^2 \) and \( \gamma \) is a scale factor.

Once the optimized depth profile is obtained, the efficiency \( Eff \) at any wavenumber in the spectrum can be calculated using Equations (4) and (5) as follows.

\[
Eff = \frac{|U_n|^2}{|U_n(0)|^2} \times 100(\%)
\]

where \( U_n(0) \) is the reflection field calculated at \( \theta = 0^\circ \) and with all \( d_m = 0 \). (In fact, \( Eff \) is not truly the absolute diffraction efficiency, which should involve an integration over allowed detection angles.)

Since the diffraction field calculation using these equations does not use Fourier transform, the number of spectrum sampling \( N \) is not necessarily restricted by the number of line elements \( M \). Therefore, the error
reduction method can improve the spectral resolution by increasing the sampling points as long as the computation capacity allows.

The objective is to find the fit parameters \( \{d_m\} \) which minimize \( \text{Err} \). When the number of parameters is fairly large as in this study, an efficient error reduction algorithm based on gradient search is essential. In the gradient search methods, the minimum is searched along the function’s conjugated derivatives direction in parameter space. The conjugated derivatives direction is determined with the current function’s negative gradient direction. There are numerous methods [10] in determining the step lengths of the fit parameters towards the minimum \( \text{Err} \).

2. Method

The spectral region of interest in this study is 725–1450 cm\(^{-1}\), in which many nerve agents, such as tabun, sarin, and soman, exhibit characteristic IR bands [11]. For their analogous target spectra, we have chosen SF\(_6\), NH\(_3\), SO\(_2\), ethylene since they can be treated with no special hazard in the laboratory. Their IR absorption spectra were obtained from database library of MIDAC Co. and used for the target spectra after normalization. This can be justified since the absorption is almost linear with (1 – transmission) when the sample concentration is very low.

Upon considering various conditions for correlation spectrometer, the micrograting size \( L \) and the diffraction angle were decided to 1.5 cm and 15\(^\circ\), respectively. Then, the highest wavenumber (\( \nu_{\text{max}} \)) in the spectral region of interest gives the width (\( \Delta \)) of the line elements, \( \Delta = \frac{1}{\nu_{\text{max}}} \text{cm}^{-1} = 13.323 \mu\text{m} \) [2]. The number of line elements is then, \( M = L/\Delta = 1126 \).

For the PRA, only 282 points were sampled from the spectral region of interest while the rest 844 points were set to zero intensity in the useless negative or lower wavenumber region. Thus, the spectral resolution upon sampling is given by \( \delta\nu = \frac{\nu_{\text{max}}}{M} = 2.58 \text{ cm}^{-1} \) [2]. For the extended PRA, the number of spectral sampling points was doubled to reduce the spectral resolution.

In the algorithms, a random phase array initiates an iterative loop of Fourier transform. The iterative loop is repeatedly re-initiated over 300 times with a fresh random phase array. After all the iterations and initiations, the phase array which gives a smallest difference between the target spectrum and the diffraction spectrum is determined to the final phase array. The final phase array is converted to the depth array of the line elements according to Equation (1), and the diffraction spectrum under the Fraunhofer approximation is synthesized using Fourier transform [2,3].

For the gradient search method, we have adopted Davidon–Fletcher–Powell (DFP) algorithm [12]. This algorithm is advantageous in applying to a large body of fitting parameters since it uses the first derivatives in updating Hessian matrix. Formulation of the DFP algorithm for the micrograting design is found in [9].

The DFP optimization begins with randomly chosen depths as the starting fit parameters. During the spectrum optimization process, the fit parameters have their variation limit within the half of the maximum wavelength. That is because the depth variation beyond the half of the maximum wavelength results in repeated interference pattern from the periodic characteristics of the interference. So, we needed to devise a unique scheme for the constrained parameters during the optimization process such that, whenever a certain depth value of line elements is increased beyond the upper limit or decreased beyond the lower limit, the corresponding depth is fixed to the near limit value. Then, the next optimization process is continued with remaining parameters excluding the fixed ones. With this special treatment of the fit parameters, we obtained the stably convergent optimization algorithm.

After the optimized depths are found, the diffraction efficiency \( \text{Eff} \) is calculated at a peak wavenumber. The optimization is repeated over 10 times with fresh random initial fit parameters. In all the repeated optimizations, the fits were excellent with small enough \( \text{Err} \) values, while each \( \text{Eff} \) value varied. The depth profile which gives the highest efficiency was chosen for the final solution.

Considering that a micrograting would be fabricated with a discrete level of depths, the calculated depths profile is quantized into 16 levels. The quality of the fit and the efficiency are degraded to acceptable degrees. Therefore, we report the results from the 16-level depth profiles.

3. Results

Figure 2(a) shows the results for SF\(_6\) obtained with the PRA and the extended PRA. The retrieved spectra show a characteristic band at 947 cm\(^{-1}\). However, a non-negligible mismatch at the band and considerable background features are obvious. Doubling the spectrum sampling points in the extended PRA did not improve the fit quality much.

Figure 2(b) shows that the DFP optimization on the same target improves the retrieved spectrum substantially. The retrieved spectrum is almost overlapped with the target spectrum. In addition, the DFP optimizations on the spectra of ethylene, SO\(_2\) and NH\(_3\) similarly result in excellent matches (Figure 3). Without doubt, the DFP optimization is successful in retrieving the target spectra.

We have also calculated the efficiencies \( \text{Eff} \) for the depth profiles obtained from the three methods. As summarized in Table 1, the \( \text{Eff} \) values for the DFP optimization are between 0.74% (SO\(_2\)) and 3.5% (SF\(_6\)). However, the \( \text{Eff} \) values for the PRA or the extended
Figure 2. SF₆ spectra generated with the PRA (red filled square), the extended PRA (blue hollow circle) in (a), and the DFP method (green hollow rectangle) in (b), compared with the target spectrum (black solid curve); $M = 1126$, $N = 563$ (extended PRA and DFP) and $N = 282$ (PRA) in 725–1450 cm$^{-1}$. (a-1) and (b-1) are the enlarged plots. (a-2) and (b-2) show the first 120 lines in the 16-level depth profiles obtained with the extended-PRA and the DFP method, respectively. (The color version of this figure is included in the online version of the journal.)

Figure 3. Spectra generated with the DFP (green filled square) compared with the target spectra (black solid curve) of ethylene, SO$_2$, and NH$_3$; $M = 1126$, $N = 563$ in 725–1450 cm$^{-1}$. (The color version of this figure is included in the online version of the journal.)
PRA are at least an order of magnitude smaller. Therefore, the DFP optimization prevails over the PRA or the extended PRA both in the fit quality and in the diffraction efficiency.

4. Discussion

There are several other approaches in designing microgratings. For example, Leskova et al. [13] presented a probabilistic approach to express the scattered field off a randomly rough surface under the Kirchhoff approximation. Belikov and Solgaard [14] used an analytical approach to describe the scattered field off a two-dimensional rough surface. In all of these approaches as well as the PRA and the DFP optimization, the Fraunhofer approximation is used to describe the diffraction field. As long as the Fraunhofer approximation holds, Equations (1)–(6) are exact and can be formulated easily into an error reduction algorithm. We have shown that programming with the DFP algorithm can be written easily and works effectively.

A useful feature in the DFP optimization would be that there is no restriction in the relation between the numbers of spectrum sampling points and line elements. The number of line elements can be increased or decreased within practical range while the spectrum sampling and the line width $\Delta$ remain same. Reducing the number of line elements while keeping the line width $\Delta$ constant downsizes the micrograting and would be favored in an optical setup where light beam collimation is a critical factor, while it results in a higher $F$ number when the diffracted beam is to be focused. While the actual micrograting size should be determined after considering such experimental aspects, we have investigated the effects on the diffraction spectra when the number of line elements is reduced.

Figure 4 shows the result for the NH$_3$ spectra retrieved from the DFP optimized depth profiles with different line numbers. As the line number $M$ is reduced, the spectrum peaks are gradually broadened and some details become obscured. In spite, the change is small that even the spectrum with as small as 500 line elements appears good enough for the correlation spectroscopy.

The success of the DFP optimization method in retrieving the target spectra provides the key to MEMS technology for fabricating the designed microgratings and to an optical setup for testing it or applying it to correlation spectroscopy. For example, a single grating with a 16-level depth profile can be fabricated with a photolithographic routine with four masks, with a submicron precision. Positioning an array of actuated micrometers and controlling their heights individually would require a higher level of expertise. In either case, how the errors in the MEMS fabrication process affect the diffraction spectrum would be a concern.

Such a concern can be addressed by applying Equations (4) and (5) to the cases when the line elements are fabricated with errors in depths or in widths. To address the effects of line depth error, Gaussian distributed errors were randomly given to the depth profiles for NH$_3$ spectrum. In the regenerated spectra (Figure 5), the major spectral feature changes negligibly but noise feature develops as the depth error ($\sigma_d$, the Gaussian

![Figure 4](image_url)
standard deviation) increases. As long as the depth error is within submicron, the correlation spectroscopy can be performed. But the greater noise feature due to larger depth error would reduce the sensitivity of the correlation.

To address the effects of the line width error in finer spectral resolution, we first generated, using the DFP optimization method, the depth profile \( \{d_m\} \) of 1126 line elements which gives a single peak at 1400 cm\(^{-1}\) (563 spectral sampling points between 1350 and 1450 cm\(^{-1}\), \( \Delta = 13.323 \) μm). Then, each line element is subdivided by \( K \) (we chose \( K = 100 \)) with all the subdivided depths \( d_{mk} \) \((k = 1, \ldots, K)\) equal to \( d_m \). Then, Equation (4) is same as

\[
U_n = \frac{1}{K} \exp(i\pi v_n \Delta \sin \theta) \sum_{k=1}^{K} \sum_{m=1}^{M} G_{mn} \exp(-i4\pi d_{mk} v_n). \tag{8}
\]

Next, a few edge sub-lines \((k = \ldots, K - 2, K - 1, K \) or \( k = 1, 2, 3, \ldots)\) of randomly chosen \( m \)th line are allowed to replace the depth with that of the edge sub-lines \((k = 1, 2, 3, \ldots \) or \( k = \ldots, K - 2, K - 1, K)\) of the neighboring \((m + 1)\)th or \((m - 1)\)th line:

\[
d_{m+1,k} \rightarrow d_{m,K+2k}. \tag{9}
\]

The replacing sub-lines \( \{m,k\} \) are selected by a Gaussian random distribution whose standard deviation \( \sigma_{mk} \) reflects the depth error deviation \( \sigma = \Delta \times \sigma_{mk}/K \).

Then, the diffraction spectrum with a given \( \sigma \) is calculated with Equations (8) and (5).

Figure 6 shows the result when \( \sigma \) is varied between 0 and 0.08Δ. For the single peak spectrum generated with \( M = 1126 \) and \( \sigma = 0 \Delta \), the main peak at 1400 cm\(^{-1}\) and the tiny ripple structures around it appear. The main peak has the broadening of 3.5 cm\(^{-1}\) at FWHM. When the width error is increased to 0.02Δ, the peak efficiency is decreased by 1.63 times while the spectrum shape is negligibly changed. As the width error is further increased, the peak efficiency is further decreased and the spectrum is distorted with grown ripple structures.

We also investigated the effect when the number of lines is reduced. In Figure 6, the black curves are the results with \( M = 700 \). Compared to the cases with \( M = 1126 \) (red curves), the spectra generated with \( M = 700 \) showed (1) broader main peak, (2) faster growth of ripple structures upon increased width error. This is contrast to the result in Figure 4. Although reducing the number of line elements by as much as twice appears to be tolerable when there is no width error, it is much more vulnerable to the width error.
The analysis implies the importance of the line width error over other factors in the micrograting design. We evaluate that the 0.04\(\Delta\) would be the upper limit of the line width error when \(M=1126\). The 4\% error corresponds to 0.53 \(\mu\)m in the width. This much tolerance would not be achievable by a typical manual aligner for photomasking in MEMS process and requires a higher precision aligner like a stepper with the typical precision of about 0.2 \(\mu\)m. When the micrograting is fabricated in multi-steps, the error from each step tends to be accumulated so that meeting the 0.53 \(\mu\)m tolerance would be barely made with the high precision aligner. The problem in meeting the line width error would be more difficult when the target spectrum is in shorter wavelength range since the 4\% error corresponds to much shorter line width error which could be beyond the current MEMS capability.

In practice, there are two kinds of MEMS microgratings: the static micrograting and the dynamic tunable micrograting. The static microgratings are fabricated with multiple masks and etching steps; the width error discussion above holds well here. The dynamic tunable microgratings are composed of an array of micromirrors, in which a gap between a neighboring pair of micromirrors is inevitable. One might be interested in the effect of fill factor in the micromirrors on the diffraction spectrum. The answer is simple; reducing fill factor is same as reducing reflectivity of micromirrors. This can be proved easily with the subdivided depth profiles and Equation (8), in which the summation is over only filled sub-lines. When the fill factor is \(r (0.5 < r < 1)\), only the efficiency is changed by \(r^2\), while maintaining the spectrum shape.

5. Conclusion
In this study of micrograting design, we have demonstrated that the error reduction method based on gradient search can be easily formulated under the Fraunhofer approximation to retrieve the target spectra precisely within experimental needs. The calculated diffraction efficiencies are much greater than those from the iterative Fourier transforming phase retrieval methods. The depth error in the micrograting line elements is calculated to affect the diffraction spectra with increased noise features while maintaining the major spectrum shape. However, the line width error affects more sensitively the spectrum shape and the diffraction efficiency. We evaluated 4\% for the upper limit of the width error for the micrograting to be applied to correlation spectroscopy. We also do not recommend reduction of the number of line elements from the current 1126 points since this would be more vulnerable to line width error.

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References