A simple and accurate wavelength calibration method for CCD-spectrometer

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Abstract: Wavelength calibration is an important step for CCD-spectrometers. The accuracy of the wavelength calibration will affect the precision of the measurement results. However, the accuracy of traditional wavelength calibration will be affected by instrument bandwidth and noise. The bandwidth of the instrument will generate the overlapping peaks in the calibration spectrum or cause the peak position shift of double peak. The noise will make inaccurate measurement of peak point. To solve this problem, a simple and accurate wavelength calibration method for CCD-spectrometer was proposed. The automated decomposition algorithm and Voigt line profile model were used to optimize the shape of the calibration spectrum and the precision value of the peak points of each calibration peak could be obtained. Using this method, the influence of bandwidth and noise could be eliminated, especially the overlap peaks could be decomposed into several single peaks, simultaneously, and the process of calibration was greatly simplified. Experiments based on USB4000 spectrometer with mercury-argon calibration light source were implemented. The results show that the proposed method could achieve higher accuracy and the calibration deviation is less than 0.1 nm. Therefore, it is recommended to use this method to calibrate the wavelength of the spectrometer.

Key words: CCD; spectrum analysis; micro spectrometer; metrology

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一种简单精确的 CCD 阵列光谱仪波长定标方法

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摘 要: 波长定标是 CCD 光谱仪的重要步骤,其准确性会影响光谱仪测量结果的精确度。然而传统波长定标精度受仪器带宽和噪声的影响:带宽会导致定标光谱中产生重叠峰或双峰的峰位移;噪声会使峰值点的测量不准确。为解决这个问题,提出了一种简单精确的 CCD 光谱仪波长定标方法。使用自动分解算法和 Voigt 线状谱模型来优化定标光谱的形状,并且可以获得每个定标峰的峰值点的精确

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值。利用该方法可以消除带宽和噪声的影响,特别是重叠峰可以被同时分解成几个单峰,极大地简化了定标过程。实施基于 USB4000 光谱仪和汞氩校准光源的波长定标实验。结果表明,相比于传统方法,该方法可以达到较高的精度且定标误差小于 0.1 nm。因此,推荐使用该方法对光谱仪进行波长定标。

关键词:CCD; 光谱分析; 微型光谱仪; 计量

0 Introduction

Spectrometers are widely used in the field of scientific researches and technology applications. By analyzing the spectrum of an object, it is easy to determine its physical properties. Before the spectrometer come into service, it is necessary to conduct wavelength calibration. Wavelength calibration includes the estimation of the peak position of some linear spectra from calibration lamp, and the fitting curve to determine the specific wavelength of all pixels.

The calibration accuracy would largely depend on two factors, the total number of lines used (more the better) and the accuracy of peak or centroid determination of reference lines recorded on the spectrometer. However, the linear spectrum measured by CCD-spectrometers usually suffers from bandwidth[1] and noise[2]. Because of the bandwidth of the instrument, it will cause overlap peaks. This reduces the number of characteristic peaks which can be used to calibration. The presence of noise makes it impossible to obtain the center wavelength of the characteristic peak accurately. So, it becomes difficult to accuracy of wavelength calibration for CCD-spectrometers.

To solve this problem, several calibration methods for spectrometer have been proposed. Sansonetti [3] et al used the smoothing algorithm and a first-derivative algorithm to deal with the linear spectrum of the mercury lamp for wavelength calibration of a Fourier transform spectrometer. Smoothing can eliminate the noise in the spectrum, and the first-derivative can enhance the resolution of the spectrum. Martinsen[4] et al used a monochromator to instead of an emission line source to generate well-separated lines, solves the problem of overlap peaks. Liu[5] et al established the analytical model of the relationship between wavelengths and pixels with the optical system parameters on the basis of geometric optics, and an accurate wavelength calibration method using the optical system parameters in proposed. Li[6] et al introduced three crucial steps for wavelength calibration such as the selection of calibration sources, the determination of the center of characteristic peak and the selection of fitting method. Sun[7] et al proposed a new calibration method which found the optimal noise reduction algorithm for processing linear spectrum at first, then the bandwidth correction algorithm is used for separation of overlapped peaks. Finally, automatic peak-seeking treatment is employed to find the center of characteristic peak. These three steps are an integral calibration process, the central wavelength of each characteristic peaks can be found more accurately.

In this paper, a wavelength calibration method base on an automated decomposition algorithm[8-10] and Voigt line profile model is proposed. This method could eliminate the effect of overlap peaks to improve the number of characteristic peaks and suppress the noise to measure the central wavelength of each characteristic peaks accurately. On the one hand, the linear spectrum measured by CCD-spectrometer is described as Voigt model. By using Levenberg-Marquardt (L-M) algorithm and the Voigt function, overlap peaks can be divided into several single peaks, the effect of overlap peaks can be eliminated. On the other hand, the proposed method uses the Voigt functions to fit the linear spectrum, the central wavelength of the peak can be obtained directly by

the parameters of the Voigt function, avoid the influence of noise. Simultaneously, the process of calibration has been greatly simplified.

The rest of paper is organized as follows. In Section 2, the Voigt line profile model for linear spectrum of spectrometer is established and the iterative process of L-M algorithm is introduced. In Section 3, the calibration algorithm is introduced in detail. Comparative experiments on USB4000 (Ocean Optics) spectrometer are presented in Section 4. Conclusions are in the Section 5.

1 Linear spectrum modeling and Levenberg-Marquardt algorithm

1.1 Linear spectrum modeling

The classical electromagnetic theory proves that the linear spectrum is a Lorentzian shape [11]. However, in fact, the spectrum measured by the CCD-spectrometer is the convolution of the spectrum itself and the instrument broadening function. Usually, the instrument broadening function of the spectrometer is described as Gauss function [12]. Therefore, the linear spectrum measured by spectrometer can be represented by Voigt function, which is the convolution of Lorentzian function and Gauss function. This relationship can be described by Eq.(1):

$$V(n)=L(n)*G(n) \tag{1}$$

where n represents the pixel number; $V(n)$ represent Voigt function; $L(n)$ denotes Lorentzian function and $G(n)$ denotes Gaussian function.

A Lorentzian function with area of S can be described as

$$L(n)=\frac{S}{\pi\gamma_L\left[\left(\frac{n-c}{\gamma_L}\right)^2+1\right]} \tag{2}$$

where S represent the area of the Lorentzian function; γ_L stands for the half-width at half-maximum(HWHM) of the Lorentzian function; c denotes the center wavelength of the Lorentzian function.

A Gaussian function with area of 1 and center wavelength of zero can be described as

$$G(n)=\frac{1}{\gamma_G\sqrt{\pi}}\exp\left[\left(\frac{n}{\gamma_G}\right)^2\right] \tag{3}$$

where $\gamma_G=\alpha_G/\sqrt{\ln 2}$, and α_G represents the HWHM of the Gaussian function. Therefore, the Voigt function can be expressed by

$$V(n;S,c,\gamma_L,\gamma_G)=L(n;S,c,\gamma_L)*G(n;\gamma_G)=$$
$$\int_{-\infty}^{\infty}L(n-n_1)G(n_1)\mathrm{d}n_1=$$
$$\int_{-\infty}^{\infty}\frac{S}{\pi^{3/2}\gamma_L\gamma_G\left[\left(\frac{n-n_1-c}{\gamma_L}\right)^2+1\right]}\exp\left[\left(\frac{n-n_1}{\gamma_G}\right)^2\right]\mathrm{d}n_1 \tag{4}$$

As a fact that the measured spectrum contains noise, the model of measured spectrum is expressed as

$$V(n)=L(n)*G(n)+N(n) \tag{5}$$

where $N(n)$ represents noise.

1.2 Levenberg-Marquardt algorithm

The proposed wavelength calibration method employs L-M algorithm. L-M algorithm is an iterative technique, where the minimum value of the evaluation function is represented as the square of the nonlinear function. The specific iterative process of L-M algorithm is as follows.

(1) With the β as variables, set the initial values to β_0, set iteration stop parameter. Calculate the error ε_k between the estimated value and actual value.

$$\varepsilon_k=y(x)-f(x,\beta_k) \tag{6}$$

where y (x) represents the actual value; f (x,β_k) represents the estimated value and k represents the number of iteration.

(2) Calculate the Jacobian matrix J_k of $f(x,\beta_k)$ on β_k

$$J_k=\frac{\partial f(x,\beta_k)}{\partial\beta_k} \tag{7}$$

(3) Construct the normal equation

$$(J_k^{\mathrm{T}}J_k+\beta_k\mathrm{diag}(J_k^{\mathrm{T}}J_k))\,\delta_k=J_k^{\mathrm{T}}\varepsilon_k \tag{8}$$

where δ_k is the correction factor.

(4) Solve the normal equation and obtain the correction factor δ_k. Add the correction factor into β_k to obtain the updated estimate

$$\beta_{k+1}=\beta_k+\delta_k \tag{9}$$

(5) Calculate the value of evaluation function with the parameters of β_{k+1}

$$e(\beta_{k+1})=\frac{1}{2}\sum(f(x,\beta_{k+1})-y(x))^2 \quad (10)$$

(6) If $e(\beta_{k+1})$ is less than iteration stop parameter, then stop iteration. Otherwise, return to step (1).

This process is implemented iteratively by replacing the new estimate instep with the updated estimate obtained in the step (4).

2 Accurate wavelength calibration method

Based on the L-M algorithm and Voigt linear model, an accurate spectral calibration method was proposed. As the model of linear spectrum has been built in Section 2, combining the L-M algorithm, we transform the issue of obtaining the central wavelength of each characteristic peaks into a multiparameter optimization problem. The evaluation function of the optimization problem is given by

$$\min e(S,c,\gamma_L,\gamma_G)=\frac{1}{2}\sum_{n_1}^{n_2}\left(\sum_{k=1}^{N}V(n;\beta)-N(n)\right)^2 \quad (11)$$

where $M(n)$ is the measured spectrum; n_1 and n_2 represent the range of pixel number; N represents the numbers of characteristic peaks and $\beta(S,c,\gamma_L,\gamma_G)$.

The details of this method are listed as follows.

(1) Acquisition of Hg-Ar lamp spectrum using CCD-spectrometer. Set the number of peaks have been fitted to $k(k=0)$ and the stop threshold T. Query the bandwidth of the CCD-spectrometer and set this value to initial value of γ_G.

(2) Let $k=k+1$. Find the maximum value of the residual spectrum v. The abscissa of the point is set to the initial value of the central wavelength c of the kth single peak. Set the initial value of $\gamma_L(k)$ to the width of the peak when the height is half. The initial value of $S(k)$ is set to the product of height and $\gamma_L(k)$. The optimal parameters of the previous $k-1$ peaks are the initial values of the kth operation.

(3) Obtain the optimal parameters of previous k single peak as well as the optimal estimated spectrum using L-M algorithm.

(4) Update the residual spectrum by subtracting estimated spectrum from original spectrum. Find the maximum value of the residual spectrum Max_k.

(5) If $Max_k>T$, return to step (2). Otherwise output the optimal parameters $c(1,2,\cdots,k)$ with the unit of pixel number.

(6) The standard wavelength and the pixel position (c) were fitted by three order polynomials, and the calibration curve was obtained.

3 Experiments on USB4000 spectrometer

To test the effect of the proposed method, experiments on USB4000(Ocean Optics) are conducted. The USB4000 is based on the Toshiba TCD1304AP linear CCD chip which contains 3 648 pixels. It is equipped with a 25 μm entrance slit and the groove spacing is 1.667 μm/line. A mercury-argon calibration light source (HG-1, Ocean Optics) is used as the calibration lamp since the wavelength range of the spectrometer is 200-900 nm. Spectra of the Hg-Ar line source were acquired using the CCD-spectrometer. The calibration spectrum is shown as Fig.1.

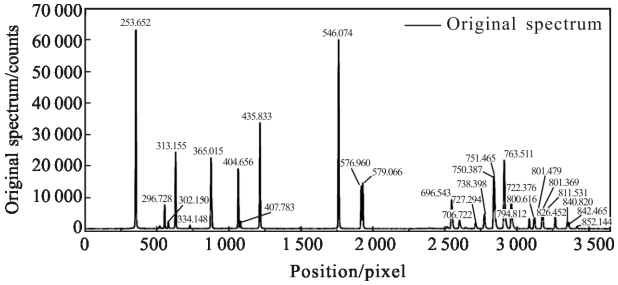

Fig.1 Spectra of mercury-argon calibration light source measured by USB4000

The first operation:

(1) The bandwidth of the spectrometer is 2 nm and pixel interval is 0.19 nm approximately, so the initial value of γ_G is set to 10.521 for each peak. The stop threshold T is set to 1 500 consider the factor of noise. Set $k=0$.

(2) $k=1$, find the maximum value of the original spectrum. Set the initial value of $c(1)$, $\gamma_L(1)$ and $S(1)$ to 351, 2.311 and 145 530, which means set $\beta_i(1)=(145\,530,351,2.311,10.521)^T$.

(3) Optimize $c(1)$, $\gamma_G(1)$, $\gamma_L(1)$ and $S(1)$ using

L-M algorithm, and obtain $\beta(1)=(162\,494,353.495,2.738,9.623)^{T}$. The first fitting spectrum is shown as Fig.2.

(4) Subtracting the first fitting spectrum from original spectrum. The residual spectrum is shown as Fig.2(b). Find the maximum value of the residual spectrum, Max_1=61 530.

(5) 61 530>1 500, return to step (2).

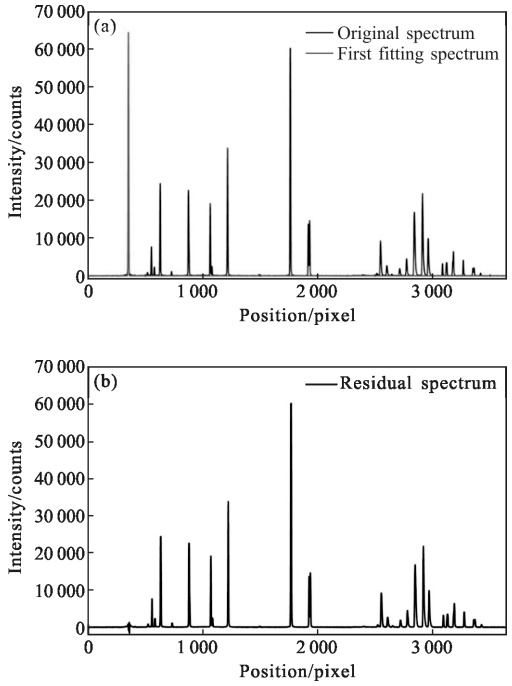

Fig.2 The original spectrum and the first fitting spectrum (a) and the residual spectrum after the first operation (b)

The second operation:

(1) k=2, set the initial value to parameters, $\beta_i(1)=(162\,494,353.495,2.738,9.623)^{T}$ and $\beta_i(2)=(150\,748,1\,760,2.452,10.521)^{T}$.

(2) Optimize these parameters using L-M algorithm. After optimization, the optimized parameters β_i $(1)=(162\,494,353.495,2.738,9.623)^{T}$ and $\beta_i(2)=(158\,621,1\,762.530,2.351,8.657)^{T}$ can be obtained. The second fitting spectrum is shown as Fig.3(a).

(3) Subtracting the second fitting spectrum from original spectrum. The residual spectrum is shown as Fig.3(b). Find the maximum value of the residual spectrum, Max_2=34 982.

(4) 34 982>1 500, return to step (1).

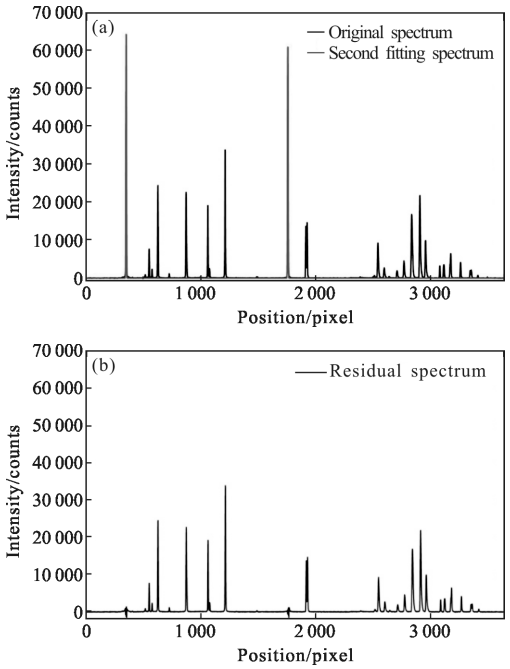

Fig.3 The original spectrum and the second fitting spectrum (a) and the residual spectrum after the second operation (b)

The 29th operation:

(1) k=29, set the initial value to $\beta_i(1),\beta_i(2),\cdots,\beta_i(29)$.

(2) Optimize these parameters using L-M algorithm. After optimization, the optimized parameters $\beta_i(1),\beta_i(2),\cdots,\beta_i(29)$ can be obtained.

(3) Subtracting the 29th fitting spectrum from original spectrum. The residual spectrum is shown as Fig.4 (b). Find the maximum value of the residual spectrum, Max_{29}=1 426.

(4) The maximum value of the residual spectrum is less than the threshold value, so the algorithm stops. The final fitting spectrum is shown as Fig.4(a).

There are two points in the algorithm need to be explained.

(1) The coefficients corresponding to the highest peak of the residual spectrum will be optimized after each operation. In the next operation, the optimal parameters of the previous peaks are treated as initial values. Finally, the optimal parameters of all peaks can be obtained. So that the central wavelength of all peaks can be obtained directly and the process of calibration has been greatly simplified.

(2) Through peaks fitting repeatedly, the overlap

peaks could be separated completely. The separation of some overlap peaks is shown in Fig.5−7. So, the total number of lines used for calibration increase.

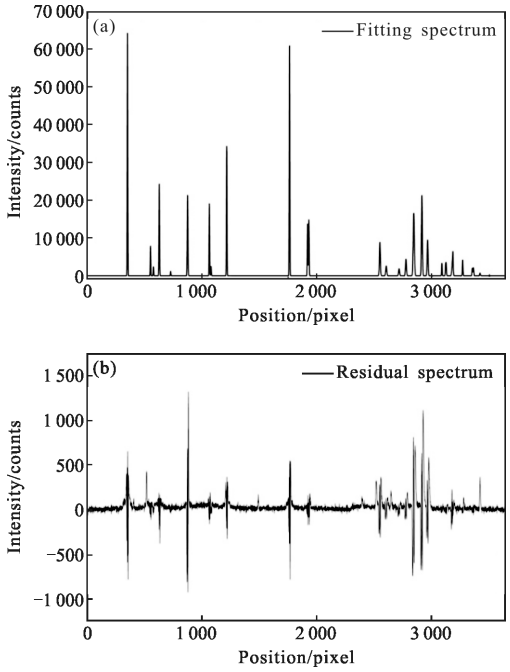

Fig.4 The final fitting spectrum after 29 times of operation (a) and the residual spectrum after the 29th operation (b)

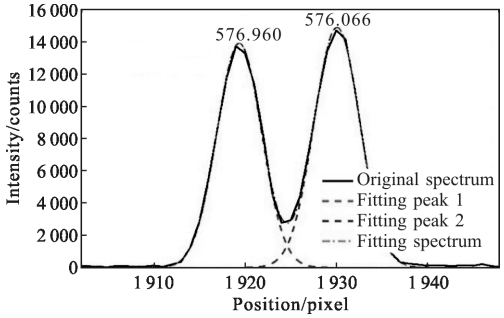

Fig.5 Original spectrum and fitting spectrum in the range of 1 900 to 1 950 pixels

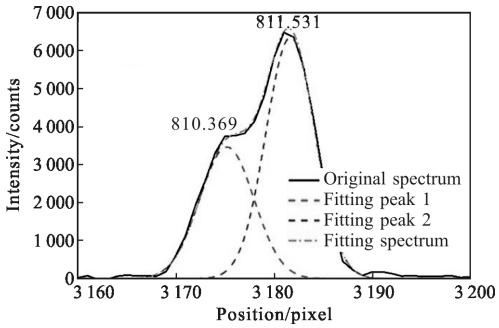

Fig.6 Original spectrum and fitting spectrum in the range of 3160 to 3 200 pixels

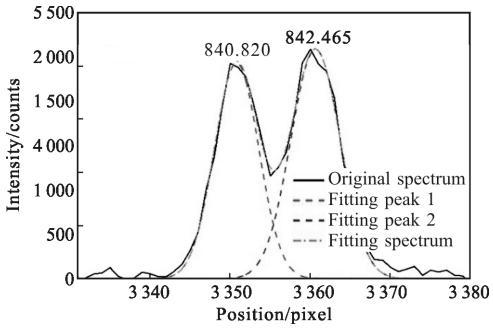

Fig.7 Original spectrum and fitting spectrum in the range of 3 300 to 3 380 pixels

The pixel positions of the 29 characteristic peaks and the corresponding standard wavelengths are listed in Tab.1. Then, the pixel positions and stand wavelength were fitted by three order polynomials. The typical relationship is shown in Fig.8, and the calibration curve can be obtained.

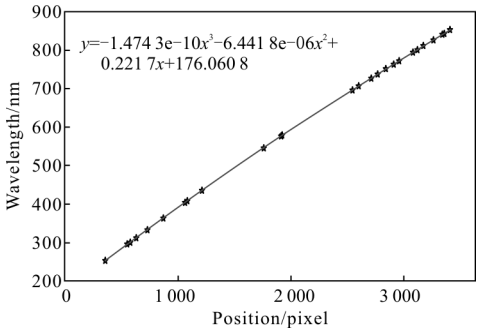

Fig.8 Typical relationship between pixel position and wavelength

Tab.1 Standard wavelength and pixel position of each characteristic peaks

Wavelength/nm	Position/pixel	Wavelength/nm	Position/pixel
253.652	353.495	738.398	2 774.865
296.728	553.650	750.387	2 840.707
302.150	578.532	751.465	2 846.713
313.155	629.929	763.511	2 913.085
334.148	728.977	772.376	2 962.573
365.015	875.250	794.818	3 087.634
404.656	1 065.222	800.616	3 120.815
407.783	1 080.181	801.479	3 125.751
435.833	1 216.193	810.369	3 175.384
546.074	1 762.932	811.531	3 182.605
576.960	1 919.966	826.452	3 267.287
579.066	1 930.882	840.820	3 350.292
696.543	2 547.755	842.465	3 359.634
706.722	2 602.798	852.144	3 415.125
727.294	2 714.188		

$$\lambda=-1.474\,3\times10^{-10}n^3-6.441\,8\times10^{-6}n^2+0.221\,7n+176.060\,8 \quad (12)$$

where λ denotes wavelength; n denotes pixel number.

To test the effectiveness of the proposed method, comparative experiments between the proposed method, Sun′s method and traditional method which use original signal to calibrate the pixel position were conducted. The calibration deviations of three methods are shown in Fig.9. The proposed method works well; the calibration deviation is less than 0.1 nm, which similar to Sun′s method. But the operation of the proposed method is simpler owing to the automated decomposition algorithm. While the calibration deviation of traditional method reaches 0.4 nm in the same situation, which proves the effectiveness of the proposed method.

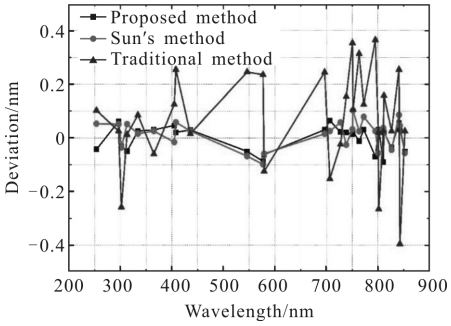

Fig.9 Calibration deviation of three methods

4 Conclusion

An approach to calibrating the wavelength scale of CCD-spectrometer has been reported. The method employs L-M algorithm and Voigt line profile model to fit the measured linear spectrum so that each characteristic peak can be calculated separately, which increase the number of characteristic peaks used for calibration and central wavelength of each peaks can be obtained accurately. Simultaneously, the process of calibration has been greatly simplified. Experiments on USB4000 with a mercury-argon calibration lamp were conducted, the calibration deviation of proposed method is less than 0.1 nm. Compared with the traditional method, more accurate wavelength calibration and easier operation can be achieved by using the proposed method.

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