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Peak Position Error Reduction Algorithm for Residual Gas Analyzer

Hun Choi*
Dep. of Electronic Eng.
Dong-eui University
Busan, KOREA

Gyeongyong Heo
Dep. of Electronic Eng.
Dong-eui University
Busan, KOREA

Jihong Kim
Dep. of Electronic Eng.
Dong-eui University
Busan, KOREA

***Abstract*— In this paper, we presents a novel algorithm that removals the peak position error due to the drift noises of a RF/DC power supply in A residual gas analyzer (RGA). The proposed algorithm is a digital signal processing technology required in developing the RGA, for reducing various noises added to the measurement data to improve the performance of the mass spectrum analysis. To reduce the additive noise (the drift noises, white noises, and etc.) in the measured data, the proposed method uses two steps of noise reduction according to the noise characteristics contained in the measurement data.**

Keywords*— Residual gas analyzer; mass spectrum; added noise; noise reduction; Block signal processing

I. INTRODUCTION

RGA (residual gas analyzer) is a generally compact, robust mass spectrometer designed for process control and contamination monitoring in vacuum systems [1]. There are two implementations that use quadrupole technology to use an open ion source (OIS) or a closed ion source (CIS) [2-4]. The RGA can be used in high vacuum fields such as research chambers, surface science setups, accelerators, scanning microscopes, and so on. RGA is useful in most cases to monitor vacuum quality and to easily detect minute microscopic impurities in low-pressure gases. These impurities can be measured up to 10 - 14 [Torr] with sub-ppm detection capability without background interference.

As shown in Fig. 1[1], the RGA can be largely divided into two parts. The first is a sensor part including the ionizer, a quadrupole mass filter, and an electron multiplier detector. And the second part is a control part which is composed of a 24V switching power supply, high voltage bias power supply for detector, RF/DC power supply for quadrupole mass filter, and MCU (main control unit) board for controlling the entire system, signal processing circuits, and monitoring system for display. The electron multiplier detector for the RGA is generally composed of a Faraday detector and electronic amplifier (the secondary electron multiplier) for measuring the ion current [1, 5].

The data obtained from the RGA is contaminated by various noises, such as the power noises occurring in different power for some units including the ionizer and the noises added to the electron multiplier detector. The various added noises degrade the ability to separate the atomic elements to represent the mass spectrum showing the composition ratio of the target gas. When analyzing a sample gas, it is especially essential for accurate qualitative analysis, and unity resolution minimizes the overlap between adjacent peaks that the peaks of different gasses are represented by the correct mass to chargeratio values, and the peaks appear at the correct positions of the corresponding ion components. Therefore, in order to develop RGA, there are necessary to develop methods for a noise reduction and a peak position tuning. However, it is very hard to remove these noises, because they are inevitably added noises which generated from the analog units (power supply, detector, pre-amp, etc.)[1, 5]

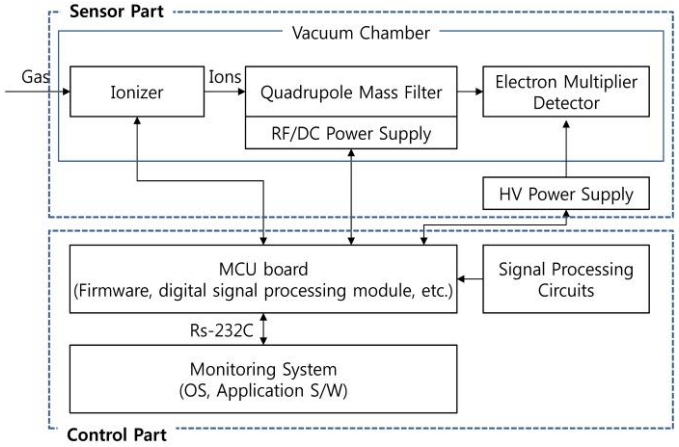

Fig. 1. Compositional diagram of residual gas analyzer[1].

In this paper, we propose a new method to remove the peak position error caused by the RF/DC power supply drift noise added to the measurement data to improve the performance of the mass analysis. The proposed method can improve the analyzing accuracy performance and analyzing speed performance of RGA, because it can perform scan process and the peak position correction at the same time, unlike the general peak tuning method that carried out before scanning for mass analysis. To evaluate the performance of the proposed method, computer simulations were carried out using a real measured data as the input.

Hun Choi : Corresponding Author*

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II. PEAK POSITION ERROR IN RESIDUAL GAS ANALYZER

The ion source of the RGA uses an electron impact ion beam that is ionized by collisions with neutral molecules or atoms as thermal electrons are generated from the filament current flow.

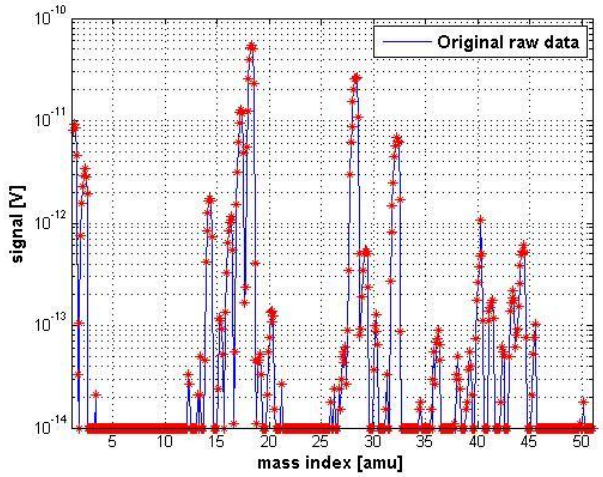

Fig. 2. The mass spectrum of the residual gas measured by the RGA under development

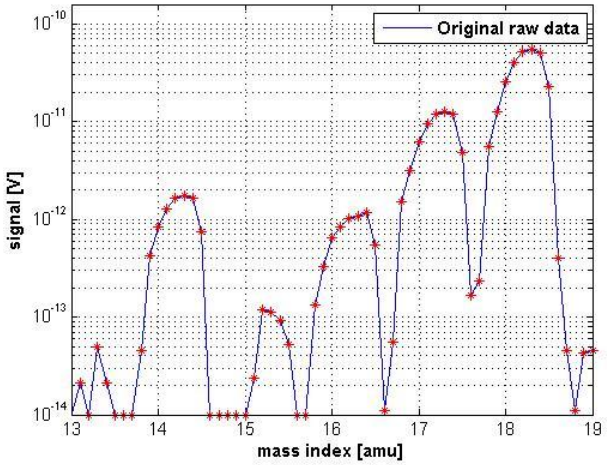

Fig. 3. Major peaks of the mass spectrum, which of the residual gas measured by the RGA under development, shifted to right due to the peak position error

The ion beam is then passed through a quadrupole mass filter. It will pass through the ions very well with the mass to charge ratio (M / e) you choose, but all other ions are pushed into the walls where they neutralize and can not be detected. The ions passing through this filter are detected as current at the Faraday detector. However, the output voltage of the RF / DC power supply for the Faraday detector may contaminate with drift noises which cause peak position errors. In the RGA analyzes the composition of the volatile substance, 1 amu resolution,

which separates the mass spectral analysis range of 1 to 100 (or 1 to 200) amu (atomic mass units) from the other peaks, is a very important specification. Fig. 2 and Fig. 3 show the mass spectrum of the residual gas measured by RGA under development (mass range from 1 to 50 amu). The data used to draw the mass spectrum is raw data that has not been subjected to data processing. Data are the original data sources obtained from the detector (Faraday detector and preamplifier) and are converted to digital data by analog to digital converter (sample rate is 10 samples/amu). As you can see, major peaks of atoms or molecules in the mass spectrum of Fig.3 shifted to right by about 3 ~ 4 samples. These peak position errors reduce the accuracy of quantitative measurement results of the corresponding mass index in mass spectrometry and interfere with the distinction from the adjacent mass index. Therefore, in order to improve the analysis performance of the RGA, it is necessary to remove the peak position error and to clearly separate the peaks of each amu.

III. THE PROPOSED PEAK POSITION ERROR REDUCTION ALGORITHM

In the RGA, after the ion signals corresponding to the atoms (or molecules) are measured by Faraday detector, they are converted to voltage signals by the pre-amp. To analyze mass spectrum using the microprocessor, the voltage signals is converted to a digital data by the ADC (analog to digital converter). When the digital-converted data obtained by the RGA defined as $s(n)$, it consists of the ion signal $v(n)$ corresponding to the atoms (or molecules) and the noise signal $u(n)$. We can express $s(n)$ as [5]

$$s(n) = v(n) + u(n) \tag{1}$$

Where n is sample index (it means the time sequence). The noise signal, $u(n)$ consists of the additional noises caused by various electric devices such as the power supply, pre-amp, and the like. In developing the RGA, a sampling frequency used in the ADC is f_s *Hz*. Assuming that the power supply noise and the pre-amp noise of a frequency higher than the sampling frequency, these noises can be changed to a drift noises with low frequency by the aliasing. Also, the drift noises contained in the output voltage of the RF / DC power supply are added to the obtained data in the process of signal detection and conversion.

To remove the peak position error, the proposed method uses two-step processes for a signal block that consists of the obtained signals. Consider the signal block that consists of the L+1 data samples, the signal block corresponding to the k-th amu is represented by

$$\mathbf{s}_k = [s(kL-L/2),\ s(kL-L/2+1),\ \ldots,\ s(kL+L/2)]^T$$

$$= [s_k(1),\ s_k(2),\ \ldots,\ s_k(L+1)]^T \tag{2}$$

where k is a positive integer and $0 \le k \le 50$.

The first step is to determine the ion signal and noise for the signal block using the quadratic curve fitting. If the signal block is a normal ion signal in (2), it will show a convex secondary curve. That is, the slop of the fitted curve with the ion signal block is positive, but that of noise signal is negative as shown in Fig. 4.

$$[slop,\ intercept] = Quad\_LS(\mathbf{s}_k) \tag{3}$$

$$if\ slop > 0,\ then\ \mathbf{s}_k\ is\ ion\ signal \tag{4}$$

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The second step is to remove the peak position errors of the ion signal block. In this step, the maximum value and the corresponding sample index are found in the signal block (the ion signal sequence), and the ion signal sequence is shifted to the left or right so that the maximum value of the signal sequence is located at the center.

$$[value\_max, index\_max] = max(\mathbf{s}_k) \quad (5)$$

$$dev(k) = index\_center - index\_max \quad (6)$$

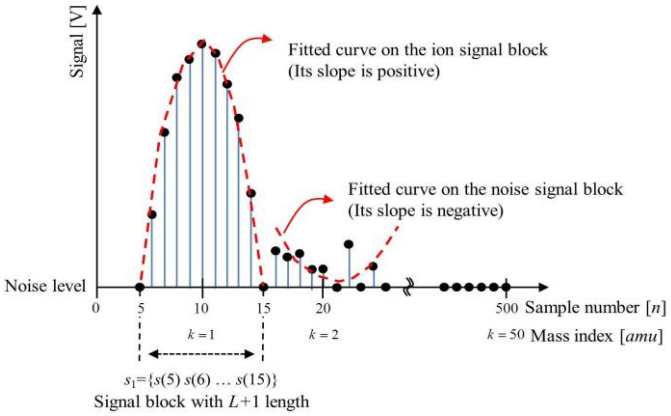
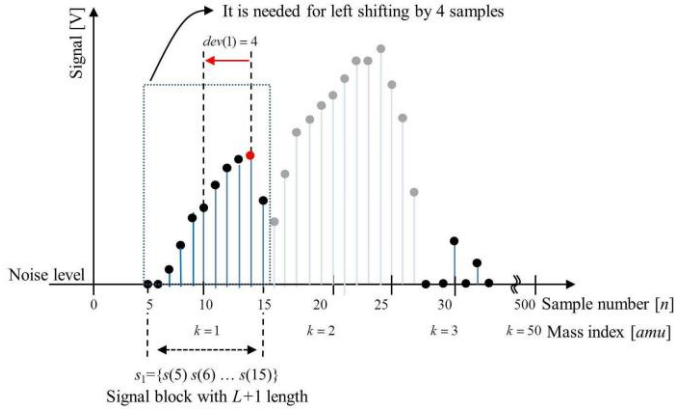
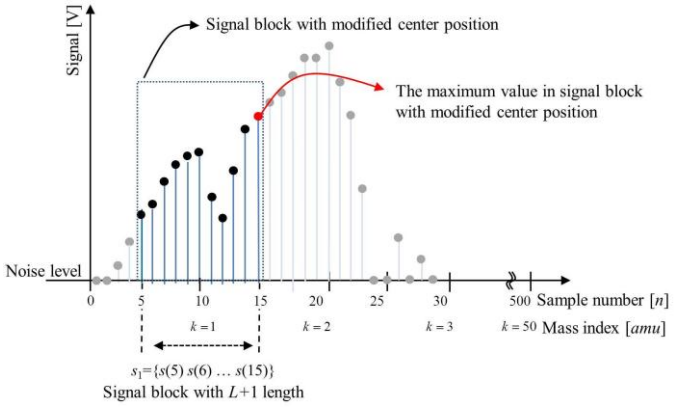


Fig. 4. Results of qudratic curve fitting on the signal block with L=10 in the mass spectrum (0 ~ 50 amu)



(a)



(b)

Fig. 5. Results of correcting center position on the (k = 1)-th signal block with $dev(1)$ = 4, (a) Before correction, (a) After correction.

where $max(\cdot)$ is a function that finds the maximum value and the corresponding sample index in the signal block corresponding to the k-th mass index(amu). The parameter $dev(k)$ is the difference of the sample index of the maximum value from the central index of the k-th signal block.

Fig. 5 shows the signal sequence before and after the correction of the center position. In Fig. 5(a), the signal sequence in the (k = 1)-th signal block is needed for left shifting by 4 samples due $\alpha + \beta = \chi.(1)$ to dev (1) (1) = 4. The sample index corresponding to the maximum value is n = 14, which is the index of the maximum value in the (k = 1)-th signal block.

Fig. 5(b) shows the result after the correction of the center position. Here, the sample index corresponding to the maximum value is n = 15. It is the index corresponding to the maximum value of data which shifted from the (k = 2)-th signal block as a result of the center position correction. However, n = 15 is wrong because it is the index of the data corresponding to the mass index (amu) = 2. To prevent from this, additional processing in performed on the center position correction following as

if $abs(dev(k)) \le \alpha L$,

else if $dev(k) > 0$, *then* $s_k(1) \sim s_k(dev(k)) = NoiseLevel$,

else if $dev(k) \le 0$, *then* $s_k(L\text{-}dev(k)+1) \sim s_k(L+1) = NoiseLevel$,

else if $abs(dev(k)) \le \beta L$,

if $dev(k) > 0$,

then $\mathbf{s}_k = [NoiseLevel, NoiseLevel, NoiseLevel, s_k(2), s_k(3) \ldots s_k(6), NoiseLevel, NoiseLevel, NoiseLevel]^T$

else if $dev(k) \le 0$,

then $\mathbf{s}_k = [NoiseLevel, NoiseLevel, NoiseLevel, s_k(6), s_k(7) \ldots s_k(10), NoiseLevel, NoiseLevel, NoiseLevel]^T$

else then $\mathbf{s}_k = NoiseLevel$.

(7)

In addition to the peak position error reduction in the proposed method, data re-arrange technique is used for improving the performance of expressing the mass spectrum to confirm the results of the residual gas composition analysis. The detailed procedure of the proposed method is shown in Fig. 6.

IV. SIMULATIONS

To evaluate the performance of the proposed noise reducing method, we carried out computer simulations with real measured signals as the input. The input signals are obtained from the RGA that is under development as shown in Fig. 1. In the RGA, Main parameters used for the quadrupole filter were

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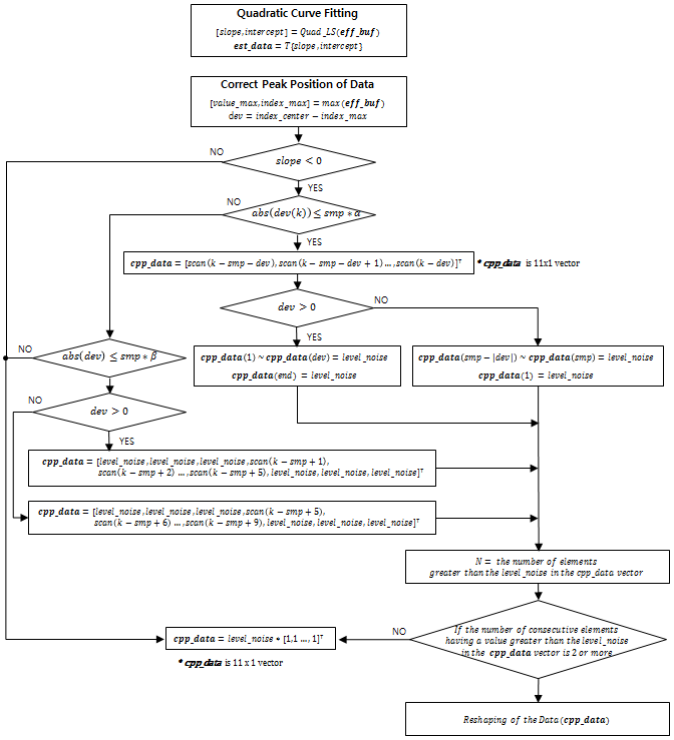

Fig. 6. Procedure of the proposed noise reducing method.

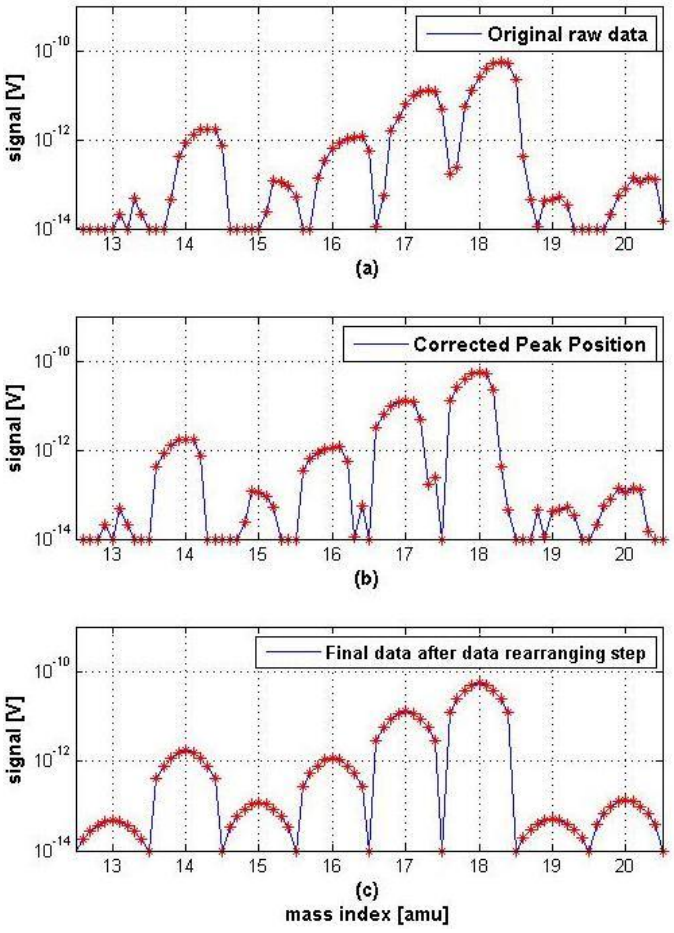

Fig. 7. Performance of the proposed method for the input signal of Fig. 2, (a) the original raw signal obtained form the RGA, (b) the result of the peak position error reduction steps, (c) the final signal after reshaping step.

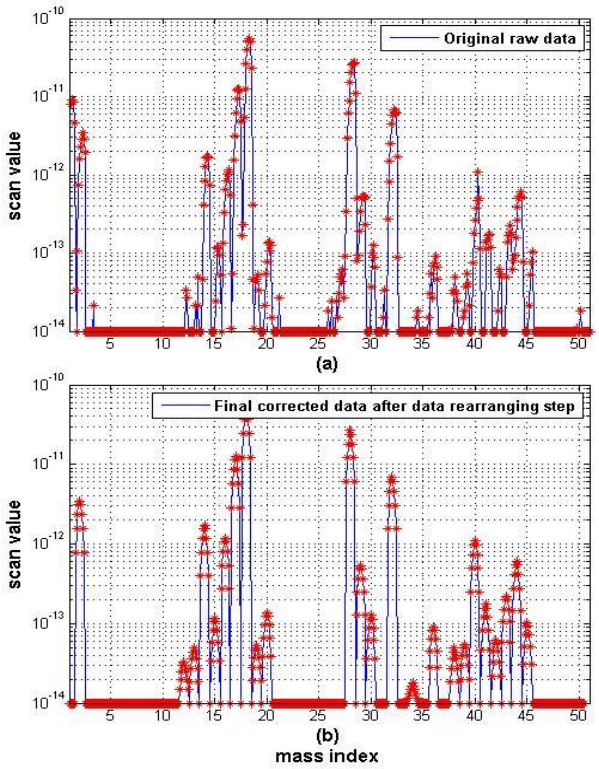

Fig. 8. Performance of the proposed method for the input signal of Fig. 3, (a) the original raw signal obtained form the RGA, (b) the improved performance in expression of the mass spectrum.

set to the electron energy is 70*eV*, the extraction is 20*eV*, and the focus is 10*eV*. Parameters for the detector were set to the pre-amp gain is 10^{-9}, the dwell time is 20μs. The scan range is 1 to 50 [*amu*] ($1 \le k \le 50$) for the mass spectrometry range. An output data rates (ODR) used for the digital data from the analog voltage signal obtained by the RGA is 10 samples/amu. The parameters used for the proposed denoising algorithm were set to the block length is $L = 10$, the noise level is $NoiseLevel = 1.0 \times 10^{-14}$, $\alpha = 3$, $\beta = 5$.

Fig. 7 shows the performance of the peak position reduction step for the mass spectrums which shown in Fig. 3. In Fig. 7(a), major peaks of atoms or molecules in the mass spectrum have some peak position errors. In Fig. 7 (a), since most signal blocks have $dev(k) = -4$, the signal sequences in each signal block require 4 samples shift to the left. Fig. 7(b) shows the performance of the proposed peak position correction algorithm using quadratic curve fitting method. The maximum values in each signal block were repositioned in the center location of the block by peak position correction. Fig. 7(c) shows the result of the post-processing which can help to clearly distinguish the peaks of the atoms or molecules from each other by reshaping of the denoised data.

Fig. 8(a) shows the mass spectrum that contaminated by a peak position errors and a number of undesirable noises. Fig. 8(b) shows the performance of the proposed algorithm with two steps. In Fig. 8 (b), the proposed algorithm has removed the peak position errors and additional noises, which appear throughout the entire mass index. As shown in Fig. 7(c), Fig. 8(b) shows a clear result of the mass spectrum.

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V. CONCLUSIONS

In this paper, we present a new peak position error reduction method for improving the mass spectrum of the RGA under development. The two processing steps that take into account drift noise and the characteristics of the white signal effectively removed various noises. In addition to, the post-processing is to be allowed to precisely distinguish between the peak of each atom or molecule by re-shaping the denoised data. Several simulation results have shown the good performance of the proposed method.

REFERENCES

[1] C.J. Park, "Operating Principle of Residual Gas Analyzer," Journ. of the Korean Vacuum Society vol.17(4), 2008, pp. 262-269.

[2] J. H. Batey, "The physics and technology of quadrupole mass spectrometers," Vacuum, 101, 2014, pp.410-415.

[3] S. Sujithra, P. Sreelatha, and S.E. Lawrence, ""Development of control algorithm for quadrupole mass spectrometer using LabVIEW," Electrinics and Communication Systems(ICECS), 2014 International Conference on. IEEE, 2014, pp. 1-5.

[4] P. H. Dawson (ed.), Quadrupole Mass Spectrometry and Its Applications, Elsevier, 2003.

[5] H. Choi and Jihong Kim, "Noise Reduction Algorithm for Residual Gas Analyzer," IJERT vol.4(11), 2015, pp. 272-276.