CORRECTION OF OVERLAPPED SPECTRAL INTERFERENCE IN ICP — AES BY SELF — MODELING CURVE RESOLUTION

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Abstract Correction of overlapped spectral lines interference in ICP—AES by self—modeling curve resolution (SMCR) is discussed, and the effect of measurement errors on resolution results is investigated. Larger effects of random errors on results are observed for closer peaks. For severely overlapped interference, use of intensities of alternate scan points which have smaller scan intervals can result in better results. Satisfactory results are obtained for correction of severe interferences.

Key words inductively coupled plasma, curve resolution, interference correction

Spectral interferences are often encountered in inductively coupled plasma atomic emission spectrometry (ICP—AES), especially in analysis of complicated samples. Various curve resolution methods have been used in the fields of chromatography, mass spectrometry etc. but have seldom been used in ICP—AES [1]. In conventional function—based methods, spectral peak is expressed approximately by some function, e. g. Gaussian or Lorentzian function, and then primary parameters such as peak height and peak width are estimated. The estimation of primary parameters is more or less arbitrary. Improper estimation of the primary parameters may result in unreasonable results. Lawton and Sylvestre [2] proposed a self—modeling curve resolution method (SMCR), which does not need assumption of peak distribution and estimation of primary parameters, and resolves a overlapped peak to separate real shapes. This method is widely used and developed.

In the present paper, a fast SMCR method proposed by Windig et al [3] is attempted to correct spectral interference in ICP—AES, and the effect of measurement errors is investigated. Satisfactory results are obtained by use of alternate intensities with smaller scan intervals.

EXPERIMENTAL

Apparatus and Working Conditions A Baird PS—3 multichannel spectrometer with 1—m Pasch—Runge mount, 1440 grooves/mm grating and a Plasma—Therm HFP 2500F rf generator (27.12 MHz, 2.5 KW) are used. Operating conditions are as follows: rf forward power 1.4 KW, outer argon flow 16 L/min, intermediate argon flow 0.85 L/min, nebulizer gas flow 0.85 L/min, observation height 15 mm above load coil, T—1.0 torch, Meinhard concentric nebulizer, and a double

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—pass spray chamber.

Data Acquisition Polyscan working mode is used to scan the profiles of analytical and interferential lines. Spectral intensity is measured once a step (1 sec. integration). For second order spectral lines, one step scan of entrance slit (5 μm) corresponds to change of 0.00166 nm in wavelength at exit slit.

Spectral intensities data are inputed to NEC PC — 8801B microcomputer (NEC Co. Japan) to perform computation. The program for computing and graphing is written with N88 BASIC.

RESULTS AND DISCUSSIONS

Effect of Random Errors Measurement may contain both systematic errors and random errors. Systematic errors result in deviation from additive spectra. Common methods of correcting spectral interferences can only be used to additive spectra. So, only the effect of random errors is discussed in the present paper.

Measurement of analytical line lanthanum 379.083 nm is interfered by holmium 379.100 nm line. In order to investigate the effect of random errors on results, simulated data with different ranges of errors are used. Results show that no significant effects are observed when errors are in the range of $\pm 10\%$ in correction of interference of 400 $\mu\text{gHo/ml}$ on determination of 1.0 $\mu\text{gLa/ml}$. However, for correcting interference of vanadium 328.939 nm line on ytterbium 328.937 nm line, random errors have more serious influence on resolution results. In resolution of 1.0 $\mu\text{gYb/ml} + 1000 \mu\text{gV/ml}$ mixture spectrum, in which errors are ranging from -3.0% to -7.7% , 0.76 $\mu\text{gYb/ml}$ and 948 $\mu\text{gV/ml}$ are obtained, which result in -24% for Yb and -5.2% for V relative errors in results. Further studies with simulated data show that when the random errors are about $\pm 1.2\%$, 0.93 $\mu\text{gYb/ml}$ and 1061 $\mu\text{gV/ml}$ are obtained, but when the random errors are about $\pm 3.0\%$, 0.65 $\mu\text{gYb/ml}$ and 1304 $\mu\text{gV/ml}$ are obtained for resolution of 1.0 $\mu\text{gYb/ml} + 1000 \mu\text{gV/ml}$ mixture, the resolved spectra seriously distort.

Resolution of Severely Overlapped Interference Attempt has been made by use of alternate intensities with 1 μm scan interval of entrance slit to correct severely overlapped interference. For the corrections of vanadium 328.939 nm line interference on ytterbium 328.937 nm, and more serious interference of neodymium 359.259 nm on samarium 359.260 nm, intensities of every five points are used for computation, and satisfactory results are obtained. Results are given in Table 1, in which the averages are as final calculating results. The original and resolved spectra are shown in Fig. 1. and Fig. 2.

It can be obtained that the real resolution of the spectrometer used in this work is about 0.0229 nm for second order spectra, and thus the spectrometer can not resolve the spectral overlaps of V 328.939 nm over Yb 328.937 nm and Nd 359.259 nm over 359.260 nm. However, when coupled with curve resolution method, the real resolution of the spectrometer can be improved by over 10—20 times, and spectral interference can be corrected.

TABLE 1. Resolution Results for Two Mixtures by Use of Alternate Intensities ($\mu\text{g/ml}$)

No.	<u>1. 0 $\mu\text{gYb/ml} + 1000 \mu\text{gV/ml}$</u>		<u>1. 0 $\mu\text{gSm/ml} + 50 \mu\text{gNd/ml}$</u>	
	Yb	V	Sm	Nd
1	1. 22	1002	0. 77	55. 8
2	1. 09	995	0. 80	57. 5
3	1. 12	978	1. 30	43. 5
4	1. 14	1053	0. 82	56. 9
5	1. 19	1035	1. 07	45. 3
average	1. 15	1013	0. 95	51. 8

Fig. 1 Spectra of ytterbium, vanadium and the mixture. Curve 1. spectrum of $1 \mu\text{gYb/ml} + 1000 \mu\text{gV/ml}$; (a) Curve 2. $1. 0 \mu\text{gYb/ml}$; Curve 3. $1000 \mu\text{gV/ml}$; (b) Curve 2, 3. resolved spectra for Yb and V respectively

Fig. 2 Spectra of samarium, neodymium and the mixture. Curve 1. spectrum of $1 \mu\text{gSm/ml} + 50 \mu\text{gNd/ml}$; (a) Curve 2. $1. 0 \mu\text{gSm/ml}$; Curve 3. $50 \mu\text{gNd/ml}$; (b) Curve 2, 3. resolved spectra for Sm and Nd respectively

CONCLUSION

Self — modeling curve resolution (SMCR) can be used to correct spectral overlap interference in ICP—AES, and to resolve components spectra from mixture spectrum. Random errors have greater influence on closer analytical and interferential lines. Satisfactory results are obtained by use of alternate intensities for correcting interferences of V 328.939 nm on Yb 328.937 nm, and Nd 359.259 nm on Sm 359.260 nm.

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