Application Note

Automatic selection of correct wavelengths

Spectral interferences in atomic spectrometry

Interferences in ICP-OES are typically cumulative and lead, in practice, to higher measurement results with neighbouring emission lines of different elements typically contributing to the signal. In the wavelength range of 200 up to 400 nm there are more than 200,000 spectral lines making manual selection of the most suitable element line in the desired concentration range very difficult. In this way, the saving in time offered by simultaneous ICP spectrometers for multi-element analysis in comparison with sequential systems is partially reduced. The selection of suitable lines for measurement is time-consuming and, accordingly, requires time-consuming post-processing of all analytical data after measurement. Shimadzu’s ICPE-9000 includes many functions that make this simultaneous ICP-OES spectrometer very easy to operate, and places special emphasis on the actual advantages of such a system: high sample throughput over a relatively narrow time window.

Wavelength selection

In sequential systems, measurements are usually carried out at the most sensitive wavelengths where spectral interferences are negligibly small if the analyte concentration is sufficiently high. In simultaneous ICP systems the selection of the optimal wavelength is far more important, as the resolution of these systems is lower compared with that offered by sequential spectrometers such as Shimadzu’s ICPS-8100. For systems with a CCD detector one should also take into account that for high element concentrations the most sensitive wavelength reaching the detector can lead to overexposure. This means that, at high concentrations, a less sensitive line may be more advantageous, which on the other hand, may be more susceptible to spectral interferences. Therefore, for analytical routine measurements it is vitally important to minimize spectral interferences for samples that are to be measured over a wide concentration range.

Automatic selection of correct wavelengths

The ICPE-9000 enables qualitative analysis of unknown samples. In this way,
it is possible to obtain an overview of all main and trace elements of the sample and, based on the line profile, to select wavelengths that exhibit suitable intensities and that are also free from spectral interferences. The selection of optimal lines can be carried out manually. However, wavelength selection via the ICPEsolution software is easier and faster. The software offers a function which supports method development and selects the optimal line for each element. In addition, it suggests the calibration range for the elements. In this way, a quantitative method can be created from a qualitative method that, with corresponding calibration standards, is tuned exactly to the samples to be measured. For very high sample concentrations causing overexposure of the corresponding lines on the detector, an alternative line can be selected retroactively from the spectrum. In this way, ICP systems with CCD detectors offer the possibility to select any wavelength retroactively to be used for post-calculation of the measuring results without the need to reanalyze the sample. This is the fundamental advantage with respect to ICP spectrometers with CID or segmented CCD detectors that only allow a limited selection of wavelengths to be added post-measurement.

The ICPEsolution software contains all element-specific wavelength information and correlative interferences as well as the associated intensities in a database and, therefore, enables reliable analyses of complex samples without any possible spectral interference.

Figure 2: Use of the interference correction standard

**Interference correction standard**

Figure 1 shows the line profile of a typical spectral interference of two neighbouring element lines of cadmium and iron. The higher the iron concentration, the stronger the cadmium signal will be affected by the additive interference. The detector records the cadmium signal at wavelength 226.502 nm as well as that of iron at wavelength 226.505 nm. The intensities of these two elements cannot be separated and an interference correction therefore needs to be carried out. The ICPEsolution software selects an additional interference correction standard measured prior to the calibration standards which compensates for spectral interferences. When a pure iron solution is measured using the cadmium wavelength of 226.502 nm, the detector will nevertheless record a signal generated only by interference of iron. This problem can easily be solved using an interference correction standard of known concentration, whereby a correction factor using different wavelengths is calculated for the intensities as described in Figure 2 for cadmium and iron. The ICPEsolution software contains all element-specific wavelength information and correlative interferences as well as the associated intensities in a database and, therefore, enables reliable analyses of complex samples without any possible spectral interference.

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