A WHITE PAPER FROM
SPECTRO ANALYTICAL INSTRUMENTS

Five reasons for upgrading to a next-generation ED-XRF analyzer

Introduction

Sometimes a difference in degree can be so great it becomes a difference in kind.

That's what's happened recently with energy dispersive X-ray fluorescence (ED-XRF) analyzer technology. The best of the newest generation of these instruments — such as SPECTRO XEPOS spectrometers, the flagship ED-XRF analyzers from SPECTRO Analytical Instruments — have seen numerous improvements that are redefining their class.

Enhancements include quantitative analysis functionality; wider analytical scope for more elements and lower concentration levels; higher sample throughput; lower cost of ownership; and greater ease of use.

This quantum leap has users rethinking what's possible with a modern ED-XRF instrument. For many applications, it matches or surpasses the performance of a more expensive wavelength-dispersive X-ray fluorescence (WD-XRF) analyzer.

This paper may be of particular interest to laboratory and quality control (QC) managers. It highlights five main reasons why upgrading to next-generation ED-XRF analyzers may be their right choice to optimize performance, efficiency, and affordability.

SPECTRO | AMETEK® MATERIALS ANALYSIS DIVISION

1. Breakthrough quantitative analysis

Traditionally, ED-XRF instruments are applied exclusively as *qualitative* analysis tools. In typical cases, a user runs samples, prints out their spectra, and compares those spectra to reference spectra of elements of interest to ensure they match. This approach most often is used as a rapid incoming *screening* tool, to quickly check whether materials of the correct chemical composition have been delivered. Most ED-XRF analyzers can indeed provide efficient, timely, relatively low-cost performance in this kind of application.

They're also used when the analysis of just a few elements in a specific matrix is required, for example in process monitoring applications.

However, this is not recommended when a large number of elements must be compared and differentiated for each sample. And this use requires an operator used to "eyeballing" comparable spectra. It takes experience to distinguish insignificant differences from visual clues that actually signal the presence of an incorrect element, and might make it necessary to reject an entire incoming shipment.

Finally, a strictly qualitative analysis can run into trouble when spectra show interference lines. In cosmetics production, for instance, the white color of a powder or cream is often obtained by including titanium oxide in the product's elemental composition. But titanium spectra can be interfered with by signals from high amounts of barium, which, when present as barium sulfate, can also produce a white color.
A qualitative analysis provides no information about the concentration of a certain element in a sample. Depending on the sample matrix and composition, spectra that look comparable may have been taken from samples with different concentrations.

New technologies have led to a revolutionary change in the nature of what's possible.

Due to improvements in excitation, detection, and calculation algorithms, new ED-XRF analyzers can also perform quantitative analysis — determining not just what elements are present, but in what concentrations, for a wide range of elements — even for completely unknown samples. SPECTRO XEPOS, for example, applies state-of-the-art software tools to identify and quantify elemental contents from sodium to uranium in unknown samples, without extensive setup.
When high accuracy is required, users simply calibrate their new ED-XRF instrument with matrix matching samples, and determine elemental compositions with unprecedented precision.

For instance, in the cosmetics processing example above, users can get a direct quantification analysis of the concentration of titanium oxide. So they know what's in the sample, and in what proportions. And they avoid sending the samples for analysis to an external lab, with attendant extra costs and delays.

Element or oxide	Unit	Analyzed conc. ± error	Certified/ recommended conc. ± error
Na_2O	%	2.68 ± 0.04	2.58 ± 0.03
MgO	%	0.752 ± 0.01	*0.49 ± 0.02*
Al_2O_3	%	13.56 ± 0.02	12.47 ± 0.06
SiO_2	%	74.30 ± 0.02	73.45 ± 0.17
K_2O	%	5.31 ± 0.01	5.00 ± 0.03
CaO	%	0.93 ± 0.002	0.84 ± 0.01
Fe_2O_3	%	2.65 ± 0.002	2.63 ± 0.02
P_2O_5	µg/g	897 ± 12	*790 ± 20*
SO_3	µg/g	2783 ±12	*2422 ± 202*
Sc	µg/g	< 3	4.1 ± 0.02
Ti	µg/g	1680 ± 4	1798 ± 18
V	µg/g	26 ± 1	25.2 ± 0.7
Cr	µg/g	48.4 ± 0.6	49.6 ± 1.7
Mn	µg/g	1211 ± 2	1038 ± 15
Co	µg/g	10 ± 4	12.4 ± 0.4
Ni	µg/g	50 ± 1	48.8 ± 1
Cu	µg/g	237 ± 2	236 ± 4
Zn	µg/g	787 ± 2	760 ± 13
Ga	µg/g	18.5 ± 0.8	17.6 ± 0.4
Ge	µg/g	0.7 ± 0.2	*1.5 ± 0.2*
As	µg/g	89 ± 2	*76 ± 5*
Se	µg/g	1.8 ± 0.2	*2.7 ± 0.5*
Br	µg/g	1.2 ± 0.2	
Rb	µg/g	147 ± 0.6	149 ± 2
Sr	µg/g	142 ± 0.4	144 ± 3
Y	µg/g	33.5 ± 0.4	32.7 ± 0.7

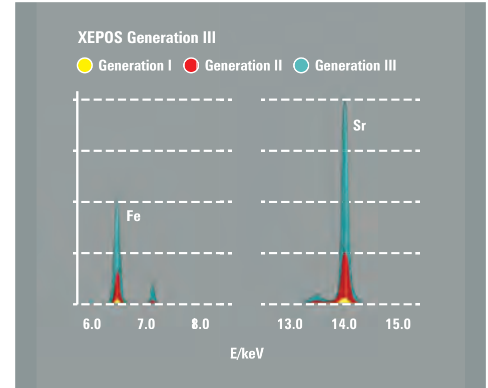
Element or oxide	Unit	Analyzed conc. ± error	Certified/ recommended conc. ± error
Zr	µg/g	232 ± 0.6	259 ± 7
Nb	µg/g	25 ± 0.4	26.2 ± 0.7
Mo	µg/g	14.9 ± 0.6	13.3 ± 0.4
Ag	µg/g	13.1 ± 0.2	*15 ± 2*
Cd	µg/g	5 ± 0.2	5.1 ± 0.2
In	µg/g	2.4 ± 0.2	*2.1 ± 0.2*
Sn	µg/g	3.7 ± 0.4	*2.4 ± 0.2*
Sb	µg/g	102 ± 0.8	*107 ± 5*
Te	µg/g	2 ± 0.4	*2.1 ± 0.4*
Cs	µg/g	4.1 ± 0.6	1.82 ± 0.1
Ba	µg/g	1012 ± 4	990 ± 12
La	µg/g	46 ± 2	46.6 ± 1
Ce	µg/g	95 ± 3	98.8 ± 1.7
Pr	µg/g	6 ± 2	11 ± 0.2
Nd	µg/g	45 ± 2	39.4 ± 0.8
Yb	µg/g	< 2	3.6 ± 0.1
Hf	µg/g	6 ± 2	7.29 ± 0.23
Ta	µg/g	< 5	1.8 ± 0.1
W	µg/g	3 ± 1	*3.5 ± 0.4*
Hg	µg/g	1.7 ± 0.4	1.44 ± 0.1
Tl	µg/g	3.9 ± 0.6	*2.8 ± 0.2*
Pb	µg/g	807 ± 2	808 ± 14
Bi	µg/g	1.6 ± 0.6	1.05 ± 0.1
Th	µg/g	15.3 ± 0.6	14.2 ± 0.4
U	µg/g	2.5 ± 0.4	2.53 ± 0.1

Table 1: Analytical results including counting statistical error (CSE) (95% confidence limit) for the metal-rich sediment SdAR-M2, prepared as pressed powder pellet using an application calibrated for the analysis of geological samples; values printed in italics are not certified

2. Added analytical capabilities

The latest-generation ED-XRF instruments have also introduced a welcome array of new analytical functionalities, including provision for analyzing more elements plus a wider range of sample concentration levels.

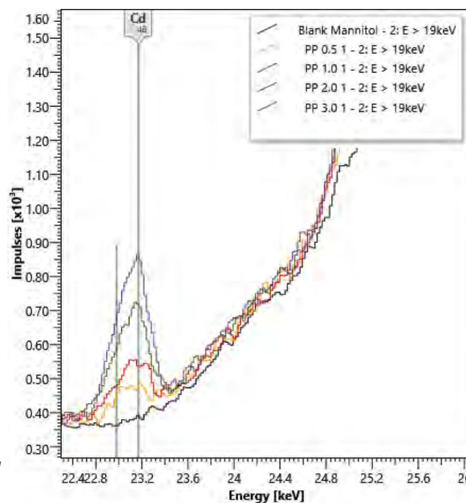
For instance, the newest SPECTRO XEPOS analyzers combine innovative detector, readout, and tube designs. These deliver unique new adaptive excitation, as well as the optimized combination of a thick binary palladium/cobalt alloy anode X-ray tube with direct excitation, excitation via a bandpass filter, and polarized excitation. Results: up to 10X greater sensitivity and up to 3X better precision than previous models. Both qualities are critical for multi-element analysis of major, minor, and trace element concentrations. So users get fast, accurate analysis of a wide range of elements in the range from sodium to uranium.

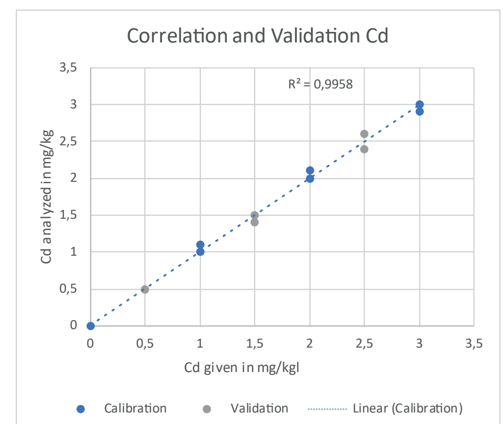


Three generations of SPECTRO XEPOS: sensitivity trending ever upward

Screening capabilities are greatly improved. With the addition of the latest unique TurboQuant II software tools, users get screening results to identify more than 50 elements in a sample. This unprecedented ability to rapidly analyze unknown samples — whether liquid, solid, or powder — means users get results for the elements they think are in the sample, plus results for elements whose presence they didn't expect, or for unwanted elements that might be detected.

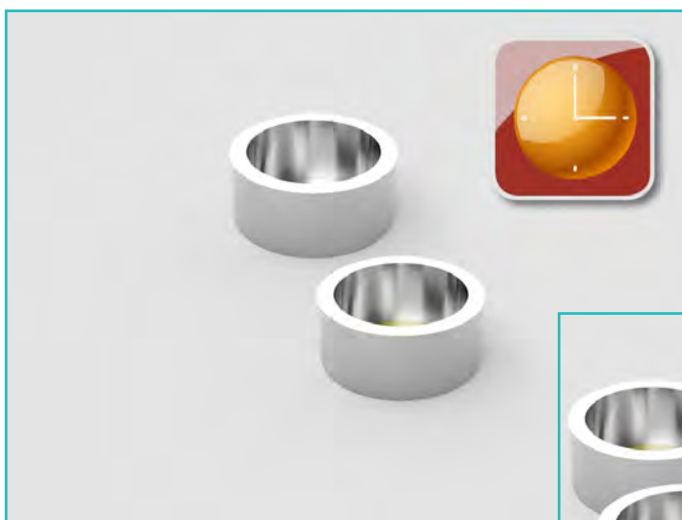
Illustration: Spectra, analysed using organic samples with nominal concentrations of 0.5, 1.0, 2.0. an 3.0 mg/kg of Cd





Higher sensitivity is another critical achievement. ED-XRF analyzer manufacturers have worked to improve sensitivity with each successive instrument generation. High sensitivity, when combined with high instrument stability, leads to high analysis precision. This is especially important when analyzing major and minor elemental concentrations.

The best new models combine high sensitivity with minimized backgrounds, realizing exceptionally low limits of detection (LODs) for that wide range of elements. If users want to go beyond screening analysis, they can now quantify elemental compositions with minor and trace element concentrations below parts per million (ppm) levels. So the instrument can be calibrated for trace elements of choice in comparable samples.



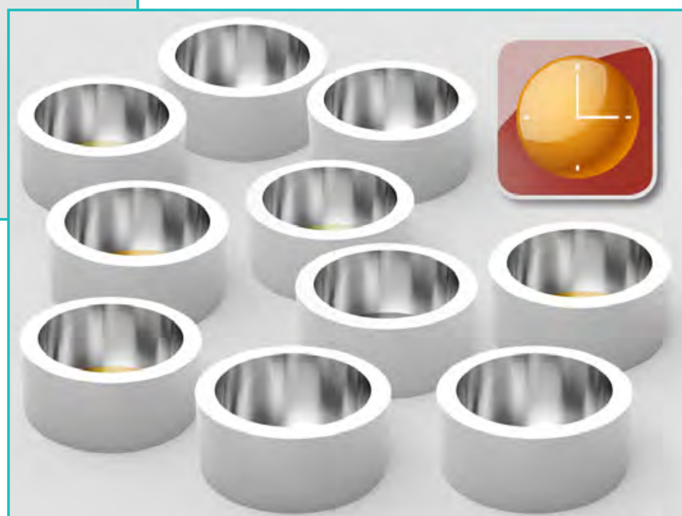


Illustration :
For many tasks, the number of samples that can be analyzed within the same measurement time is significantly higher compared to previous ED-XRF models.

Until now, obtaining such precision and detection limits with an XRF instrument would typically have required the use of a WD-XRF analyzer — often at more than twice the purchase price of today's ED-XRF models.

3. Greatest sample throughput

For numerous users, their applications and workflows mandate that an analyzer deliver both high sample throughput and short measurement times. Until recently, in the universe of XRF spectrometers, this combination was the exclusive domain of WD-XRF instruments. However, advancements such the new high-sensitivity detection system of SPECTRO XEPOS, with its significantly enhanced count rate, mean that this level of performance is now possible with an ED-XRF instrument as well.

In fact, with these technologies, analysis times can be cut dramatically.

For many simple tasks, measurement can be completed within just a few seconds. Returning to the previously mentioned

cosmetics example, in the past it might have taken 3 minutes to analyze a sample for the presence of various elements. The best new instruments can now perform the same analysis in only 30 seconds!
Even a comprehensive screening, which took 20 minutes with previous ED-XRF models, can now be completed in only 2 minutes or less.

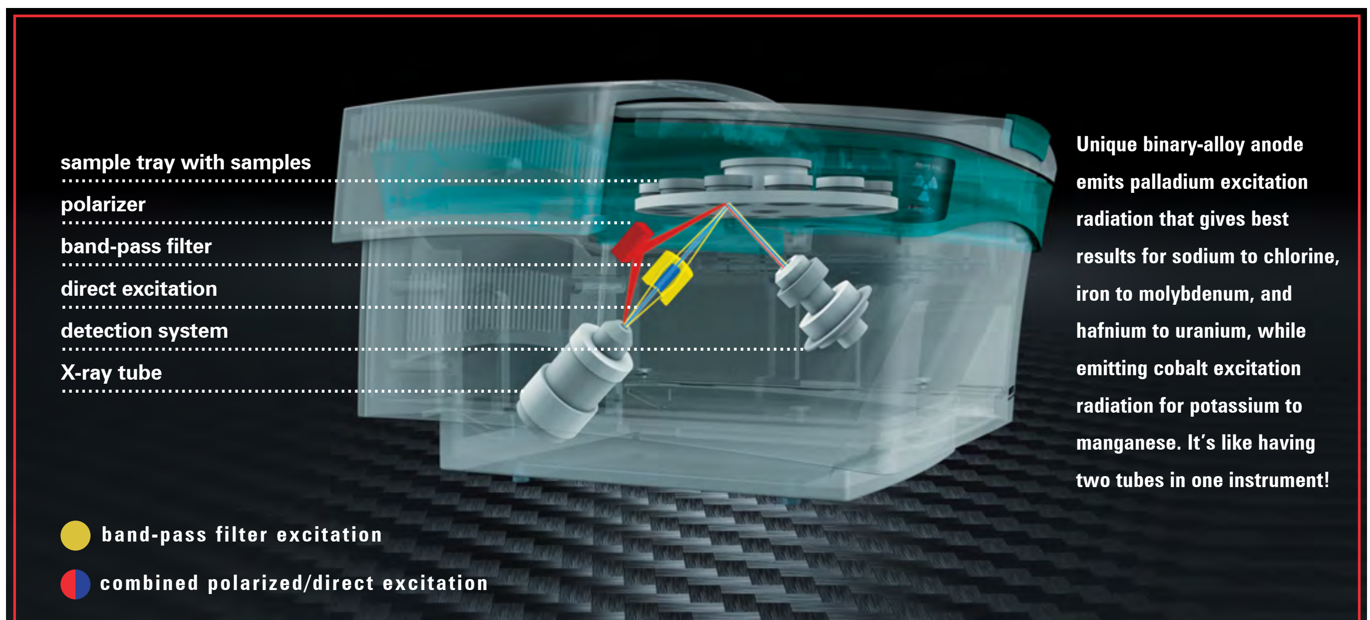
Note that when productivity rate is less critical, the user may prefer to take longer for the sake of greater precision. In addition, extending measurement time to 10 minutes, for example, would in many cases permit true quantification analysis of trace elements down to sub-ppm levels.

This flexibility could let a large organization dedicate some instruments to the highest possible throughput, and others to the greatest precision or lowest detection limits. A smaller laboratory might choose to perform screening analyses for most of a busy day, then enter the same samples and run a trace element analysis during a break, or at night.

4. Lower cost of ownership

An advanced ED-XRF analyzer such as a new-model SPECTRO XEPOS still exhibits significantly lower costs — of initial investment and long-term operation/ownership — than WD-XRF spectrometers. Yet with the gains in analytical power this class of instrument has made in recent years, it can provide comparable performance for many applications.

Unlike most WD-XRF analyzers, it offers lower power consumption (only 200 W). It can provide a long component life cycle — typically 5 to 7 years. When components finally must be replaced, they're often less costly: for example, a new SPECTRO XEPOS tube is around a third of the cost of a high-power WD-XRF tube.



Finally, its consumption flexibility adds even more savings. Instead of constant purging of liters of expensive helium, helium purging (at low volume) is used only when required for analysis of concentrations of light elements in liquids and powders, while a vacuum system is used when analyzing solid samples.

To maximize their savings, users should closely consider their needs. Any new instrument purchase should be carefully matched to the level of performance they actually require.

Challenging applications or advanced specifications could demand the full capabilities of the flagship SPECTRO XEPOS spectrometer. However, those with much more easily satisfied requirements might prefer a solution such as the portable yet powerful SPECTROSCOUT analyzer — or even the newly upgraded SPECTRO xSORT handheld analyzer. Given the technological improvements in ED-XRF classes already mentioned, an affordable modern handheld like the latter may well equal or exceed the performance of many older benchtop XRF models.

5. Ensured ease of use

Across a variety of organizations worldwide, laboratory managers report that their technicians may be required to operate as many as five different instruments on a routine basis. Each device possesses its own learning curve. Technicians must familiarize themselves with multiple aspects of setup, operation, and maintenance to achieve mastery.

Over time, top manufacturers have made continuous efforts to simplify operator

interactions with each succeeding iteration of ED-XRF instruments. The new generation offers the greatest ease of use yet.

For example, with SPECTRO XEPOS, users may request their own application-specific configurations, or choose from an array of optional packages precalibrated for common applications. Workflow and sample handling are made flexible and convenient. Advances include a versatile new measurement chamber, which accommodates larger or irregularly shaped samples and accepts an optional 25-position sample tray for automated productivity. And the analyzer's operating software interface has been redesigned and optimized — with third-party user input and testing — to be powerful, intuitive, and exceptionally easy to learn and use.

Conclusion

ED-XRF technology has made great strides in recent years. Now more than ever, not all analyzers are created equal.

Laboratory managers should consider their current instruments, and review the new functionality — such as quantitative performance, additional analytical capabilities, increased throughput, lower cost of ownership, and greater ease of use — that the best new ED-XRF analyzers can offer.

The right choice may provide such decisive advantages that the choice to upgrade becomes inevitable.

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