PRODUCT SPECIFICATION No. 41117

QuantAS™: Quantitative analysis using scans

Powerful XRF semi-quantitative analysis package for ARL 9900 Series and ARL PERFORM'X Series WDXRF spectrometers

QuantAS is an analytical software package for Thermo Scientific X-ray fluorescence spectrometers. QuantAS offers powerful semi-quantitative analysis capabilities and is fully integrated within OXSAS, the main software driving the instrument and analytical functions.

Introduction

In general, semi-quantitative programs are very useful when:

(a) No or very few suitable standards are available to perform a true calibration program for a specific matrix type

(b) Various types of samples have to be analyzed which do not fit into any particular calibration program

(c) Totally unknown samples or "ad hoc" samples or non-routine samples have to be characterized etc.

Both solids and liquids can be analyzed using QuantAS. The QuantAS program works in conjunction with the universal gearless XRF goniometer and therefore can be fitted on both ARL PERFORM'X and ARL 9900 Series instruments. The gearless goniometer has the analytical flexibility and versatility to exploit the virtues of X-ray fluorescence for most of the elements from Beryllium to Uranium.

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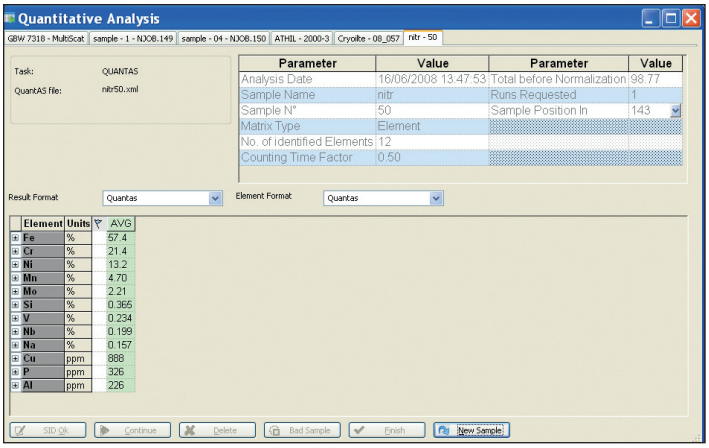

Figure 1. QuantAS report: Example of the result screen.

Figure 2. ARL PERFORM'X Series.

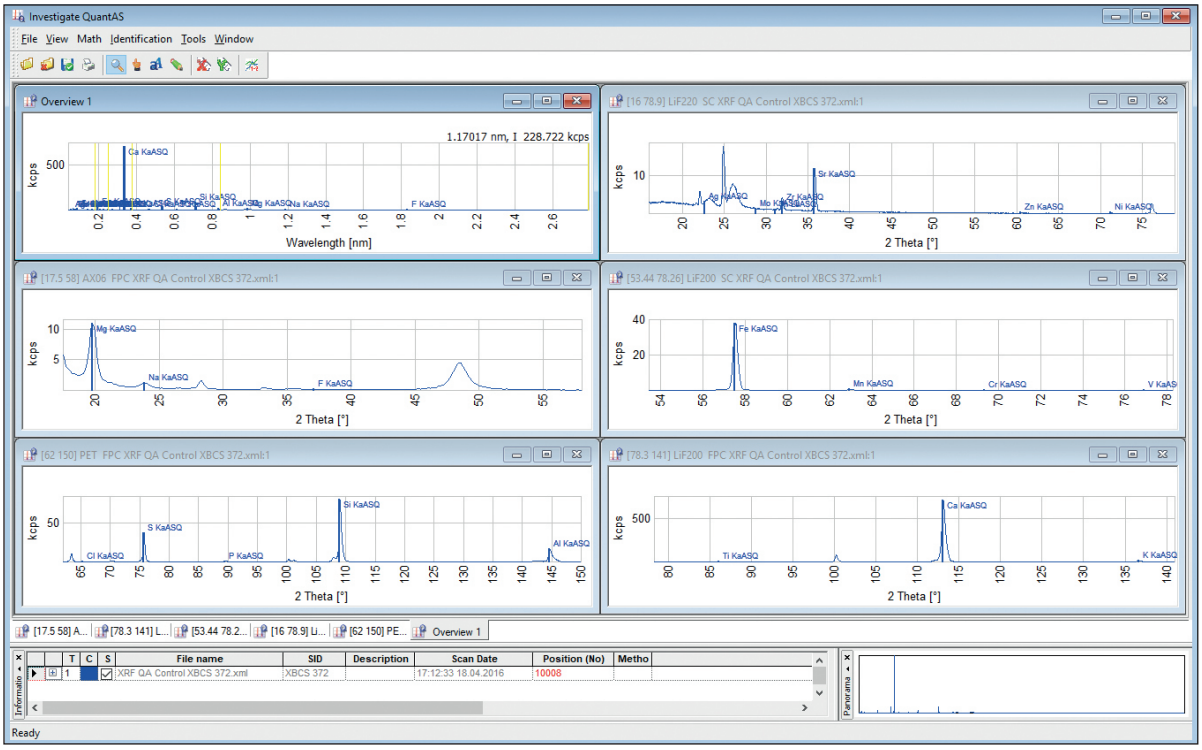

Figure 3. Processing through graphics can be automatic or manual.

QuantAS takes this analytical capability to a further dimension by quantifying the elemental or oxide composition of the sample without conventional calibrations. In addition, both ARL PERFORM'X and ARL 9900 Series can be fitted with large capacity X-Y autosampler to handle a wide variety of samples in batch mode or unattended operation mode.

Table 1. Salient features of QuantAS

	Feature	QuantAS
1	What can be analyzed?	Regular solids, liquids, loose powders (irregular solids and thin films)
2	How does it work?	Acquisition of scans followed by spectral processing
3	Element coverage	Fluorine to Uranium (except Ru, Rh)
4	Matrix coverage	Elements, Oxides, Fusion beads, Binders, %Rest
5	Analysis time	From 3 to 12 minutes typically Programmable up to ~20 h
6	Scan graphics	Global and individual scan graphics with many interactive features
7	Special features	"Type standardization" for better accuracy: creation of standards library for finger printing: ideal for plastics, oils, special alloys, thin films etc.
8	Film and He factors	Mylar or PP film or He correction factors included for loose powders and liquids
9	Performance	Better accuracy for majors and minors, excellent detectability of traces, elements reported down to several ppm
10	Configuration required	LiF220, LiF200, PET, AX06 crystals, fine collimator on the universal gearless goniometer
11	Recalibration	Simple and direct method using 4 multi-element glass standards
12	Software integration	Total integration under OXSAS

The QuantAS program is based on scans followed by spectral processing. The following bullet list explains the different steps involved in processing the acquired scans into concentrations.

- Smooth spectrum
- First search for elements
- Calculate backgrounds and subtract from the peak intensities
- Second search for elements
- Calculate overlaps and subtract from peak intensities to get net intensities
- Apply COLA model using pure intensities, net intensities and alpha factors (Fundamental Parameters)
- Apply correction for film thickness and He environment if used
- Apply type standardization if used
- Calculate concentrations
- Normalize result

Typical examples of QuantAS analysis

Table 2. Analysis report: BS 162 maraging steel.

Element	Concentrations	
	Given	QuantAS
Fe	31.2%	30.5%
Ni	21.8%	22.1%
Cr	21.6%	21.9%
Co	17.8%	17.8%
Mo	2.83%	2.86%
W	2.38%	2.39%
Mn	0.910%	0.941%
Ta	0.752%	0.790%
Si	0.382%	0.414%
Al	0.134%	0.240%
La	265 ppm	280 ppm
Ti	232 ppm	270 ppm
V	Unknown	180 ppm
Cl	Unknown	170 ppm
Ca	Unknown	120 ppm
K	Unknown	110 ppm
Cu	206 ppm	110 ppm
Nb	110 ppm	59 ppm
P	112 ppm	12 ppm

Table 3. Analysis report: Pure Al.

Element	Concentrations	
	Given	QuantAS
Al	99.5%	99.5%
Mg	0.023%	0.102%
Si	750 ppm	920 ppm
Fe	650 ppm	510 ppm
Cu	300 ppm	470 ppm
Ti	370 ppm	450 ppm
Zn	230 ppm	380 ppm
V	370 ppm	370 ppm
Ni	300 ppm	370 ppm
Mn	300 ppm	320 ppm
Cr	280 ppm	270 ppm
Sn	100 ppm	130 ppm
Pb	98 ppm	130 ppm
Ga	70 ppm	58 ppm
S	Unknown	28 ppm
Zr	Unknown	10 ppm

Table 4. Analysis report: BNRM CDA 863, Cu alloy.

Element	Concentrations	
	Given	QuantAS
Cu	64.3%	64.2%
Zn	25.3%	25.2%
Al	5.10%	5.18%
Mn	2.82%	2.67%
Fe	2.23%	2.10%
Ni	0.200%	0.288%
Cl	Unknown	0.110%
Si	<100 ppm	760 ppm
S	4 ppm	520 ppm
P	<100 ppm	310 ppm
Pb	180 ppm	240 ppm
Ca	Unknown	63 ppm
Cr	Unknown	30 ppm

Table 5. Analysis report: NIST 195 ferro-silicon (pressed with 20% Methyl-Cellulose).

Element	Concentrations	
	Given	QuantAS
Si	75.3%	75.1%
Fe	23.6%	24.3%
Mn	0.17%	0.16%
Cl	Unknown	740 ppm
Al	650 ppm	650 ppm
Ca	530 ppm	540 ppm
Mg	Unknown	530 ppm
Cu	470 ppm	520 ppm
W	Unknown	510 ppm
Cr	470 ppm	430 ppm
Ni	320 ppm	420 ppm
Ti	370 ppm	370 ppm
Zr	110 ppm	160 ppm
Mo	Unknown	54 ppm
Zn	Unknown	36 ppm
S	10 ppm	31 ppm

Table 6. Analysis report: NIST 1886, cement.

Element	Concentrations	
	Given	QuantAS
CaO	67.4%	66.9%
SiO_2	22.5%	22.0%
$Al2O_3$	3.99%	4.99%
SO_3	2.04%	3.14%
MgO	1.60%	2.09%
Fe_2O_3	0.310%	0.30%
TiO_2	0.190%	0.202%
K_2O	0.160%	0.177%
SrO	0.110%	0.128%
P_2O_5	250 ppm	150 ppm
V_2O_5	Unknown	140 ppm
Cr_2O_3	<100 ppm	94 ppm
MnO	130 ppm	88 ppm
ZrO_2	Unknown	26 ppm
ZnO	<100 ppm	23 ppm
NiO	Unknown	14 ppm
MoO_3	Unknown	2 ppm

Table 7. Analysis report: NIST 97b, clay.

Element	Concentrations	
	Given	QuantAS
SiO_2	42.4%	45.7%
Al_2O_3	39.2%	40.2%
TiO_2	2.39%	2.44%
Fe_2O_3	1.19%	1.24%
K_2O	0.618%	0.707%
MgO	0.187%	0.297%
SO_3	Unknown	0.117%
CaO	348 ppm	740 ppm
ZrO_2	~675 ppm	690 ppm
P_2O_5	~458 ppm	590 ppm
V_2O_5	Unknown	370 ppm
Cr_2O_3	332 ppm	340 ppm
BaO	~222 ppm	160 ppm
SrO	99 ppm	120 ppm
ZnO	~108 ppm	110 ppm
Ga_2O_3	Unknown	76 ppm
Nb_2O_5	Unknown	70 ppm
NiO	Unknown	66 ppm
MnO	61 ppm	57 ppm
PbO	Unknown	55 ppm
Cl	Unknown	45 ppm
Rb_2O	Unknown	35 ppm
Y_2O_3	Unknown	33 ppm
CuO	Unknown	20 ppm

Table 8. Analysis report: NIST 88b, dolomite.

Element	Concentrations	
	Given	QuantAS
CaO	30.0%	29.7%
MgO	21.0%	23.9%
SiO_2	1.13%	2.25%
Al_2O_3	0.34%	1.02%
Fe_2O_3	0.277%	0.274%
K_2O	0.103%	0.187%
SO_3	Unknown	0.184%
Cl	Unknown	0.118%
TiO_2	~160 ppm	220 ppm
MnO	160 ppm	170 ppm
Na_2O	290 ppm	98 ppm
P_2O_5	44 ppm	96 ppm
SrO	76 ppm	77 ppm
NiO	Unknown	6 ppm
Rest (CO_2)	46.37%	42.30%

Table 9. Analysis report: GBW07311, sediment.

Element	Concentrations	
	Given	QuantAS
SiO_2	76.3%	76.0%
Al_2O_3	10.4%	13.4%
Fe_2O_3	4.39%	4.32%
K_2O	3.28%	3.55%
MgO	0.620%	0.748%
CaO	0.470%	0.444%
Na_2O	0.460%	0.401%
TiO_2	0.350%	0.355%
MnO	0.321%	0.300%
SO_3	424 ppm	800 ppm
PbO	685 ppm	700 ppm
Rb_2O	446 ppm	520 ppm
P_2O_5	584 ppm	510 ppm
ZnO	464 ppm	480 ppm
Cl	290 ppm	330 ppm
SnO_2	420 ppm	320 ppm
BaO	321 ppm	280 ppm
As_2O_3	248 ppm	210 ppm
ZrO_2	207 ppm	170 ppm
WO_3	159 ppm	130 ppm
CuO	98 ppm	100 ppm
V_2O_5	84 ppm	61 ppm
Sb_2O_3	19 ppm	60 ppm
Y_2O_3	54 ppm	59 ppm
Bi_2O_3	56 ppm	57 ppm
Nb_2O_5	36 ppm	37 ppm
SrO	34 ppm	34 ppm
NiO	18 ppm	23 ppm
Ga_2O_3	25 ppm	22 ppm

Table 10. Analysis report: SARM 42, soil.

Element	Concentrations	
	Given	QuantAS
SiO_2	74.1%	64.0%
Al_2O_3	10.0%	16.1%
Fe_2O_3	4.68%	4.51%
MgO	1.92%	1.92%
CaO	0.890%	0.879%
Cr_2O_3	0.630%	0.556%
K_2O	0.450%	0.519%
TiO_2	0.360%	0.347%
SO_3	0.050%	0.126%
MnO	1000 ppm	860 ppm
Na_2O	~1500 ppm	670 ppm
P_2O_5	~400 ppm	650 ppm
ZrO_2	259 ppm	230 ppm
BaO	~308 ppm	200 ppm
NiO	159 ppm	180 ppm
Cl		150 ppm
V_2O_5	168 ppm	150 ppm
ZnO	55 ppm	56 ppm
SrO	44 ppm	45 ppm
Co_3O_4	48 ppm	41 ppm
Rb_2O	24 ppm	21 ppm
CuO	21 ppm	17 ppm
PbO	~11 ppm	15 ppm
SnO_2		3 ppm
Rest (H_2O)		10.70%

Table 11. Analysis report: BCS 372, cement (Fusion 1:12).

Element	Concentrations	
	Given	QuantAS
CaO	65.8%	66.3%
SiO_2	21.3%	19.1%
Al_2O_3	5.35%	5.72%
Fe_2O_3	2.49%	2.67%
SO_3	2.350%	2.650%
MgO	1.300%	1.780%
K_2O	0.620%	0.591%
TiO_2	0.330%	0.328%
Na_2O	0.210%	0.323%
SrO	0.170%	0.200%
P_2O_5	0.190%	0.164%
MnO	600 ppm	560 ppm
Cl		430 ppm
V_2O_5		200 ppm
NiO		190 ppm

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Table 12. Analysis report: BCR 40, coal.

Element	Concentrations
	QuantAS
Si	2.05%
Al	1.42%
S	0.968%
Fe	0.576%
K	0.333%
Cl	0.227%
Na	0.131%
Ca	990 ppm
Mg	980 ppm
Ti	700 ppm
Ba	130 ppm
Mn	66 ppm
V	49 ppm
P	39 ppm
Sr	24 ppm
Ni	21 ppm
Cu	20 ppm
Cr	19 ppm
Rb	19 ppm
Pb	16 ppm
Zn	15 ppm
Nb	1 ppm
Rest (C)	93.9%

Table 13. Analysis report: Standard 1, polypropylene.

Element	Concentrations	
	Given	QuantAS
Al	46 ppm	48 ppm
Ca	28 ppm	39 ppm
P	18 ppm	29 ppm
Cl	20 ppm	21 ppm
S		20 ppm
Si		18 ppm
Ni		7 ppm
Rest (CH_2)		99.9%

Find out more at **thermofisher.com/oxsas**

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