SPECIFICATION

Rigaku / X-ray Fluorescence Spectrometer

Optional Programs of ZSX Guidance

Software Specifications

Rigaku Corporation

Contents

1. Preface

This specifications document describes the details of useful optional programs for the operation software on Rigaku sequential WDXRF spectrometers. The optional programs in this document are currently available in ZSX Guidance software on ZSX Primus IVi, ZSX Primus IV, ZSX PrimusIII+, ZSX Primus400 and Supermini200 and also available in ZSX software on ZSX Primus and ZSX PrimusII.

2. Optional programs of ZSX Guidance

2.1. SQX Program

Function:

A qualitative scan is run, and the detected elements are then quantified by the fundamental parameter (FP) method without the use of reference standard samples. In the quantifying process, a sensitivity library is used which has the FP sensitivities for all elements that can be analyzed by XRF and which has been calibrated using pure metals and reagents.

Features:

- EZ Scan — Just by inputting several conditions, SQX can be performed for unknown samples.
- Fixed-angle measurement function — It is possible to add fixed-angle measurement in SQX analysis. Using this function, the X-ray intensity is collected at a fixed 2θ angle for a user defined given time, usually much longer than the time for a step in scanning; therefore, precision is greatly improved and superior results can be obtained for trace element analysis.
- Thin-film FP — The FP method is employed in SQX quantification. In the process of theoretical X-ray intensity by the FP method, not only concentration of each element but also weight per area (or thickness) of the sample can be considered. Therefore, it is possible to apply SQX to film, coating (single layer/substrate), filter and sample whose thickness is not enough. When the sample amount is too small to make a pressed briquette with sufficient thickness, SQX can be applied.
- Automatic theoretical overlap correction — In SQX, theoretical X-ray intensity, calculated from the chemical composition (and sample thickness) by the FP method, is used to correct spectral overlapping. This correction is automatically applied; it is not necessary to manually apply peak deconvolution to separate peaks in peak overlapping.
- Various corrections — SQX includes the following corrections:

- Alpha or beta lines
- Measurement area (sample size)
- Tube current
- Attenuator
- Photoelectron FP (for O, N, C and B)
- Sample film (for liquid or loose powder)
- Impurity (blank subtraction)
- Helium atmosphere

SQX can be applied to various samples or materials. It is not necessary to create library sensitivity for each material or application.

- Drift correction sample set — SQX Program option includes a drift correction sample set. This sample set is measured when the library sensitivity is established at Rigaku factory. By running this sample set, it is possible to update the library sensitivity for drift correction.

Typical samples/applications:

Non-routine samples or totally unknown samples

2.2. Matching Library (Function)

Function:

The program automatically selects the standard sample with the concentrations the closest to the sample to be analyzed from the standard samples registered in Matching Library. The FP sensitivity of the selected standard sample is used for FP calculation in SQX analysis. It is possible to register reference materials or house standards the user owns in Matching Library.

Features:

The selected standard sample, whose matrix is similar to the unknown sample, is used for SQX calculation as sensitivity library; therefore, it is possible to perform more accurate analysis using Matching Library because error factors caused by the sample matrix, particle size and mineralogical composition, are offset.

Typical samples/applications:

Metal and alloy, geological material such as ore, rock or mineral

Notes)

- Matching Library is available when SQX Program is ordered.
- Matching Library option is just a function. Matching library sensitivity data is not included in this option.

2.3. SQX Scatter FP Method

Function:

Scatter lines (Rh-Kα Compton and Thomson) derived from the X-ray tube are used in the FP method of SQX calculation to estimate the influence of components which cannot be / are not analyzed in SQX (e.g. H, B, C, N, O).

Features:

In the FP calculation of SQX, each concentration value is normalized as the total concentration is 100 mass%. If information of components that cannot be analyzed by XRF is not input, the resultant values are incorrectly normalized. Therefore, in such a case, it is necessary to set the balance component, whose concentration is calculated by subtracting the total concentration of the other components from 100 mass%.

However, there are some cases where it is difficult to set the balance component, such as for waste plastic or oil, soil, sludge.

Using SQX Scatter FP Method, it is possible to obtain accurate results for samples for which it is difficult to set the balance component.

Typical samples/applications:

Plastic, waste oil, geological material, solution, soil, fly ash, sludge

Notes)

- SQX Scatter FP Method is available when SQX Program is ordered.
- For liquid samples, SQX Scatter FP Method can be applied only for ZSX Primus.
- The crystal LiF(220) is required except for Supermini200.

2.4. Material Identification

Function:

This program looks up the material standards registered in the program and shows (and print out) the standard matched to the SQX result. The standards of ASTM and JIS for aluminum alloy, copper alloy, iron and steel are registered.

User specified compositions can also be additionally registered for identifying in-house materials.

Typical samples/applications:

Steel and alloy

Notes)

Material Identification is available when SQX Program is ordered.

2.5. Quant. Scatter FP Method

Function:

In quantitative analysis, this program can calculate theoretical intensity of scatter lines.

(1) When the scatter ratio method (Compton scatter ratio or background ratio method) is applied in empirical calibration, the program calculates theoretical alphas for calibration.

(2) In quantitative analysis by the FP method, the program calculates background intensities for analysis samples, so that it is not necessary to measure background intensities, which shortens the total counting time.

Typical samples/applications:

- Heavy elements in geological material such as ore, concentrate
- Oils (C/H and O correction, Lite Matrix Correction)

Notes)

(1) for empirical calibration function

2.6. Quantitative Theoretical Overlap Correction

Function:

In quantitative analysis by the FP method, theoretical intensities can be used for overlap correction, instead of measured intensities.

Features:

When there is an absorption edge between a correcting line and overlapping line, overlap correction does not work well because the intensity of the correction line is not proportional with the overlapping line. To avoid the above situation, theoretical intensity, which is calculated with consideration of absorption and enhancement by co-existing elements, is used for overlap correction.

In addition, it is not necessary to measure the element whose line is an overlapping line; for example, an overlapping line is an element of the balance component or the substrate of a layered sample.

Typical samples/applications:

Steel and alloy, coated or multi-layered sample

Notes)

- This program is just for quantitative analysis by the FP method (FP calibration).
- This function is different from theoretical overlap correction in the SQX.

2.7. Fusion Bead Correction

Function:

This program can calculate theoretical alphas for fusion beads to correct for error factors in the fusion method.

Features:

- LOI/GOI correction — In the calculation process of theoretical alphas, the program eliminates the effect of LOI (loss on ignition) or GOI (gain on ignition); therefore, it is not necessary to determine LOI/GOI (i.e. ignite sample) in advance.
- Dilution ratio correction — The program calculates the theoretical alpha for flux, so that the deviation of the dilution ratio (flux to sample in weight) from the standard ratio can be corrected by specifying actual flux and sample weights for each bead. With this dilution correction, it is not necessary to precisely weigh the flux and sample, even it is possible to apply “catch weight” for weighing the flux and sample.
- Flux evaporation correction — In the case of some fluxes (e.g. sodium borate), the flux is evaporated during fusion, which causes deviation of the actual dilution ratio from the designed dilution ratio. This correction considers evaporation of flux and so enables accurate analysis by the fusion method even with flux evaporation, by inputting the weight of sample and also the weight of the bead.

Typical samples/applications:

Geological material, such as ore, rock or mineral, oxide, such as cement, refractory, ceramics

2.8. Charge Correction Program

Function:

Based on the analysis results, the program calculates the amount of each raw material to be added into the charge in order that the concentration of each element in the charge should be within the standard. Raw material is not necessary to be pure metal.

Simplex method is used to calculate the amounts to be added in order that the cost should be minimized.

Typical samples/applications:

Steel and alloy making, raw meal for cement

Notes)

Microsoft Excel is used for the calculation.

2.9. Automatic Program Operation

Function:

(1)Time Preset Analysis — A series of analyses are automatically run at a time or interval specified. For example, PHA adjustment and measurement of drift monitor samples are automatically measured at 7:00 every morning.

(2)Energy Saver — When measurement is not performed for given time, the program automatically reduces kV and/or mA or turns off X-ray.

(3)Automatic Power-off — The program automatically turns off X-rays or the main power after analysis is finished.

Notes)

- “Tube-aging”, which automatically increases X-ray power after turning on X-rays gradually, is included in the standard software of ZSX Primus series.
- For Supermini200, only (1) is available.

2.10. Reporting Program for Hazardous Element Analysis

Function:

A qualitative application including fixed-angle measurements of Cd, Pb, Hg, Cr and Br is provided. A sample is measured by SQX using this qualitative application, and then an analysis report about these hazardous elements is made by one-click in SQX Analysis.

Features:

This program is targeted to Cd, Pb, Hg, Cr and Br, the object elements for WEEE, RoHS and ELV Directives. The report includes qualitative charts and analysis values of these elements.

Typical samples/applications:

Hazardous elements for WEEE, RoHS and ELV Directives

Notes)

- Reporting Program for Hazardous Element Analysis is available when SQX Program is ordered.
- Microsoft Office is required.

2.11. LIMS Command Receiving Function

Function:

This program reads an analysis request file created by LIMS (Laboratory Information Management System) computer and then automatically sets sample ID's based on the content of the file.

Notes)

A function to transmit analysis result data to LIMS computer is included in the standard software.