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Principle and Performance of Portable X-Ray Fluorescence (XRF) Analysis for Rock Geochemical Characterization Using Bruker S1 Titan 600

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Abstract Portable X-Ray Fluorescence (pXRF) is widely used for rapid, non-destructive geochemical characterization of rocks and soils in laboratory and field applications. This study evaluates the working principles and analytical performance of the Bruker S1 Titan 600 portable XRF analyzer for rock-derived materials. Construction fill soil and iron sand samples collected from Aceh Province, Indonesia, were analyzed using the geomining calibration mode under controlled laboratory conditions with repeated measurements. The results show that silicon (Si) is the dominant element in construction fill soil, with concentrations consistently exceeding 60 wt%, while iron (Fe) is dominant in iron sand samples with concentrations above 70 wt%. The repeated measurements demonstrate good analytical repeatability for major elements, indicating that the instrument is suitable for preliminary geochemical classification and screening of geological materials.

1. Introduction

Geochemical characterization of rocks and soils is a fundamental process in mineral exploration, environmental monitoring, and geotechnical assessment. Conventional analytical techniques such as Inductively Coupled Plasma–Optical Emission Spectroscopy (ICP-OES) and Atomic Absorption Spectroscopy (AAS) provide high analytical accuracy but require complex sample preparation and laboratory-based analysis (Kurniawan dan Wahid, 2025). As an alternative, X-Ray Fluorescence

(XRF) offers rapid, non-destructive, and multi-elemental analysis with minimal sample preparation, making it suitable for both laboratory and field applications (Nurhayati, 2023).

Recent developments in portable XRF (pXRF) instrumentation have significantly improved detector resolution and analytical speed, enabling real-time geochemical screening during exploration activities (Nengsih et al., 2024). The Bruker S1 Titan 600, equipped with a Silicon Drift Detector (SDD), has been widely applied in geomining investigations due to its robustness, portability, and reliable elemental quantification of major and minor elements in geological materials (Widyatmoko, 2010). The purpose of this study was to evaluate the working principle and analytical performance of the Bruker S1 Titan 600 portable X-Ray Fluorescence (pXRF) instrument in the geochemical analysis of rock-based materials. The evaluation was carried out through repeated measurements of construction fill soil and iron sand samples to assess the consistency of the results, the repeatability of the measurements, and the ability of the instrument to identify and classify materials based on the composition of major elements.

2. Theoretical Background

2.1 Principle of X-Ray Fluorescence

X-ray fluorescence (XRF) is an elemental analysis technique based on the interaction between high-energy X-rays and matter. When a material is irradiated with primary X-rays, inner-shell electrons of atoms may be ejected if the incident energy exceeds their binding energy. The resulting vacancies are filled by electrons from higher energy shells, leading to the emission of characteristic X-ray photons. The energies of these photons are unique for each element, allowing qualitative identification, while their intensities are proportional to elemental concentrations, enabling quantitative analysis.

2.2 X-Ray Generation in Bruker S1 Titan 600

In the Bruker S1 Titan 600 portable XRF analyzer, X-rays are generated using an X-ray tube equipped with a tungsten target. Electrons emitted from a heated filament are accelerated toward the anode under high voltage, producing X-rays upon impact. The generated radiation consists of bremsstrahlung radiation, which forms a continuous spectrum, and characteristic radiation resulting from electronic transitions within the target atoms. Tungsten is selected as the target material due to its high atomic number and high melting point, which ensure stable X-ray production under high thermal and electrical operating conditions.

2.3 Detection System: Silicon Drift Detector (SDD)

The Bruker S1 Titan 600 employs a Silicon Drift Detector (SDD), which provides high energy resolution and fast signal processing. The SDD enables accurate discrimination between closely spaced elemental peaks, significantly improving analytical reliability compared to earlier proportional or PIN detectors. This feature is crucial for complex geological matrices where spectral interferences are common.

2.4 Matrix Effects and Analytical Limitations

XRF measurements are influenced by matrix effects, including absorption and enhancement phenomena caused by the surrounding elemental composition. These effects can alter fluorescence intensities and introduce systematic errors. To minimize such influences, the Bruker S1 Titan 600 utilizes factory-calibrated algorithms and application-specific modes (e.g., geomining mode), which incorporate empirical and fundamental parameter corrections.

3. Materials and Methods

3.1 Instrumentation

Elemental analyses were conducted using a Bruker S1 Titan 600 portable XRF analyzer equipped with an SDD detector and integrated Bruker Elemental Analysis Software. Measurements were performed in both laboratory (stationary) and field (handheld) configurations.

3.2 Sample Preparation

Rock-derived samples consisted of construction fill soil and iron sand collected from selected locations in Aceh Besar Regency, Aceh Province, Indonesia. Samples were air-dried to remove moisture and homogenized prior to analysis. No chemical treatment was applied, consistent with the non-destructive nature of XRF analysis.

3.3 Measurement Procedure

Samples were placed on the measurement window and shielded using the detector safety cover. The geomining calibration mode was selected, and each sample was measured three times with an acquisition time of approximately 60 seconds per measurement to evaluate precision and repeatability.

4. Results

4.1 Elemental Composition of Construction Fill Soil

The results of the portable XRF analysis are presented to evaluate the elemental composition and measurement repeatability of construction fill soil samples. Three repeated measurements were conducted under identical conditions to assess analytical consistency. The elemental composition of construction fill soil obtained from Lamtadok, Aceh Besar, was analyzed using the Bruker S1 Titan 600 portable XRF analyzer in geomining mode. To evaluate measurement precision and repeatability, each sample was measured three times under identical laboratory conditions. The results of the XRF analysis are summarized in Tables 1–3.

Tabel 1. Elemental composition of construction fill soil (Test 1) measured using Bruker S1 Titan 600

Element	Mean Concentration (%wt)	Standard Deviation (%wt)
Si	33.7	7.2
Al	8.5	0.5
Fe	6.6	0.5
Ca	4.1	0.2
Mg	2.8	0.2
K	2.0	0.2
Na	1.3	0.1
Mn	0.48	0.03
Cu	0.12	0.01
Zn	0.10	0.01

Silicon (Si) is the dominant element in the construction fill soil samples, with an average concentration of 33.7%wt, indicating the predominance of silicate minerals such as quartz and feldspar. Aluminum (Al) and iron (Fe) also show relatively high concentrations, reflecting the presence of aluminosilicate and iron-bearing mineral phases. The calculated standard deviations for major elements are relatively low compared to their mean values, suggesting good repeatability of the Bruker S1 Titan 600 measurements under laboratory conditions.

Minor elements such as Mn, Cu, and Zn exhibit low concentrations with small standard deviations, indicating stable detection performance despite their lower abundance. Overall, the statistical summary demonstrates that repeated pXRF measurements yield consistent elemental data, supporting the reliability of the instrument for rapid geochemical screening applications. The summarized statistical values presented in Table 4 provide a clear comparison of elemental abundances and measurement variability; therefore, additional graphical representation was considered unnecessary.

4.2 Instrument Configuration and Measurement Geometry

Figure 1 illustrates the main components of the Bruker S1 Titan 600, including the X-ray tube, Silicon Drift Detector (SDD), measurement window, and shielding system.

Figure 1. Main components of the Bruker S1 Titan 600 portable XRF analyzer

5. Discussion

The elemental composition results obtained using the Bruker S1 Titan 600 portable XRF demonstrate consistent detection of major elements in rock-derived samples; however, several analytical factors must be considered when interpreting the data. In pXRF analysis, measurement accuracy is influenced not only by instrumental performance but also by sample-related effects and physical limitations inherent to X-ray interactions.

5.1 Sources of Analytical Error

Potential sources of error in pXRF measurements include surface heterogeneity, particle size variation, and sample positioning relative to the detector window. Because the analysis was performed without chemical digestion or pelletization, variations in grain size and surface roughness may cause localized differences in X-ray absorption and scattering. These effects can lead to minor fluctuations in measured elemental concentrations, particularly for elements present at low levels. Instrumental drift and counting statistics may also contribute to uncertainty; however, the low standard deviation values observed for major elements indicate that such errors are minimal under controlled laboratory conditions.

5.2 Matrix Effects in pXRF Analysis

Matrix effects play a significant role in XRF analysis, as the presence of multiple elements within a sample can influence both excitation efficiency and fluorescence yield. High concentrations of silicon and aluminum in the construction fill soil samples may result in absorption or enhancement effects that affect the detection of lighter or trace elements. In pXRF systems, these matrix interactions are partially corrected through factory calibration models, such as the geomining mode used in this study. Nevertheless, residual matrix effects may still influence quantitative accuracy, particularly for elements with overlapping spectral lines or low fluorescence energies.

5.3 Detection Limits of Portable XRF

The detection limits of pXRF instruments are generally higher than those of laboratory-based XRF or ICP-based techniques, especially for light elements and trace metals. In this study, major elements such as Si, Al, Fe, Ca, and Mg were reliably quantified, while minor elements exhibited lower concentrations approaching the practical detection limits of the instrument. The stable detection of minor elements with low standard deviation suggests that the Bruker S1 Titan 600 is suitable for semi-quantitative to quantitative screening; however, for precise trace element analysis, complementary laboratory methods may be required.

5.4 Implications for Geological Screening Applications

Despite these limitations, the results confirm that pXRF provides a rapid and reliable tool for preliminary geochemical characterization. When combined with appropriate calibration modes and controlled measurement conditions, the Bruker S1 Titan 600 offers sufficient analytical performance for geological screening, material classification, and quality control purposes. Understanding the influence of analytical error sources, matrix effects, and detection limits is essential to ensure proper interpretation and responsible use of pXRF data in applied geoscience studies.

6. Conclusion

This study demonstrates that the Bruker S1 Titan 600 portable X-ray fluorescence (pXRF) analyzer is an effective tool for rapid, non-destructive elemental analysis of rock-derived materials under controlled laboratory conditions. The instrument successfully quantified major elements such as Si, Al, Fe, Ca, and Mg with good repeatability, as indicated by low standard deviation values from repeated measurements. The analysis confirms that pXRF is well suited for preliminary geochemical screening and material characterization, particularly for applications requiring fast data acquisition and minimal sample preparation. However, the interpretation of pXRF results must consider potential sources of analytical error, matrix effects, and instrument detection limits, especially when assessing minor and trace elements. Overall, the Bruker S1 Titan 600 provides reliable and consistent elemental data for geological screening purposes, while complementary laboratory-based techniques are recommended for detailed quantitative trace element analysis.

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Author Contributions

AF performed data analysis and prepared both the original and revised versions of the manuscript. MR contributed to the preparation of the original manuscript and its subsequent revisions.

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