X-Ray Fluorescence Spectroscopy (XRF)

Technical White Paper



Introduction

X-Ray Fluorescence Spectroscopy, otherwise known as XRF, is an analytical technique which is used to establish the composition of a range of materials including metals, minerals, fluids and sediments. XRF technology has advanced considerably in recent years and is now a commonly used piece of portable equipment which has been specifically designed to determine the presence and percentage of a range of elements in the range of 100 % to sub-ppm-level.

XRF analysis is especially useful if the sample needs to be analysed non-destructively as most other techniques will require sectioning or burning of the sample to identify the chemical composition. XRF is also useful for onsite testing where the samples cannot come to the laboratory.



The analyser mounted in a frame for the analysis of small samples in the laboratory.



History

A physicist named Wilhelm Conrad Roentgen is acknowledged for his accidental discovery of X-rays. This took place in 1895 whilst conducting an analysis on cathode rays in high voltage, discharge tubes containing gas. However, a way of using X-rays for analysis was not established by Roentgen, but rather, it was a man named Henry Moseley who discovered a way to implement X-rays into an analysis technique. Moseley derived a mathematical equation regarding the relationship of the wavelength of an X-ray photon and the specific atomic number of an element. The first scientists to use primary X-rays in 1925 were named Dirk Coster and Yoshio Nishina.

The initial demonstration of the use of X-Ray Fluorescent Spectroscopy began really in the 1960's with development in the 1970's of affordable, accurate, highly advanced pieces of equipment. These were initially large laboratory-based instruments but following the development of small-scale X-ray tubes, these can now be made into small, portable, hand-held instruments that have proven to be one of the most useful analytical methods of today.

How X-Ray Fluorescence Spectroscopy works:

1. An x-ray beam (the primary x-ray) is generated within the analyser and directed at the test sample.



External Stimulation Created by XRF

- 2. The primary x-ray beam then interacts with the atoms in the sample by displacing electrons from the inner orbital shells of the atom. This effectively occurs as a result of the difference in energy between the primary x-ray beam emitted from the analyser and the binding energy that ensures that the electrons remain in their proper orbits; the displacement happens when the x-ray beam energy is higher than the binding energy of the electrons with which it interacts.
- 3. Electrons are fixed at specific energies in their positions in an atom, and this determines their orbits. When electrons are dislodged out of their orbit, they leave behind vacancies, which then makes the atom unstable. The atom must immediately correct the instability by filling the vacancies that the displaced electron's left behind. Those vacancies can be filled from higher orbits that move down to a lower orbit where a vacancy exits.
- 4. The further away the electrons are from the nucleus of the atom, the higher the binding energy. Therefore, an electron will lose some energy when it drops from a higher electron shell to an electron shell which is closer to the nucleus. This change in energy is accounted for by emission of secondary x-rays, termed as fluorescence. The amount of energy lost is equivalent to the difference in energy between the two electron shells. This is determined by the distance between them. The distance between the two orbital shells is unique to each individual element.



5. The fluorescent x-ray energies are unique to each element and can be used to identify the element from which it emanates. In order to determine the quantity of each element present, the proportion in which the individual energies appear can be calculated by the instrument. The entire fluorescence process occurs in small factions of a second. A measurement using this process with a modern handheld XRF gun can be made in a matter of seconds. The actual time required for a measurement will depend on the nature of the sample and the levels of interest. High percentage levels will take a few seconds while part-per-million levels will take a few minutes.



Handheld X-ray fluorescent (XRF) analysers have the capability to quantify nearly any element from Magnesium to Uranium, depending on specific instrument configurations. Portable XRF spectrometers allow you to take the battery operated analyser to the sample rather than bringing the sample into the lab. This is especially useful when the test specimen is large and heavy or needs to be analysed in-situ.



Applications and Capabilities:

The analysis of metals and alloy components to determine chemical composition to ensure the sample conforms to the specification.

To gain information on an unknown sample and to establish the material grade.

The XRF has the ability to analyse geochemistry samples to aid mineralogy investigations into the chemical composition of an 'earth' material e.g. limestone analysis.

XRF analysis can be used to determine the lead percentage in paint.

Analysis of shavings and turnings.

The XRF offers RoHS Screening to determine the presence of the five core substances that are restricted by regulations which are lead (Pb), cadmium (Cd), mercury (Hg), chromium (Cr) and bromine (Br).

Bulk analysis of homogenous powder samples.

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