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Use of XRD in the Iron Ore Business

By Karsten Knorr, Bruker AXS GmbH, Karlsruhe, Germany, and Ning Yang, Bruker AXS, Beijing, China

X-ray diffraction, or XRD, is the only analytical method that directly measures the mineralogy of ore. Ore is considered a rock mass from which one or more minerals or metals can be recovered at a profit. This article outlines the use of XRD for the qualitative and quantitative mineralogy of iron (Fe) ores.



In the iron ore business, the amount and type of the iron-bearing species in the ore (e.g. hematite, magnetite, goethite, and others) is measured for general quality and grade control of the run-off mine material.

Ore components that have no commercial value – the gangue – have to be removed as much as feasible. Knowing the gangue minerals and their composition (e.g. silica and alumina from clay, mica, feldspar or others; carbonates) determines the necessary steps of beneficiation (washing, magnetic or gravity separation) before further processing of the ore. Furthermore, selective mining of the most profitable material is made possible by identifying regions of low- or high-grade ore in the mine.

XRD is used to detect iron-bearing mineral impurities that are difficult to process. Wuestite (FeO), for example, is commonly found in technical products such as mill scales. Although having the highest Fe content of all iron minerals, it is not wanted in raw iron production due to technological reasons.

The bulk chemical composition can be calculated from the concentration of the minerals and their known stoichiometry, similar to X-ray fluorescence or XRF, but without element calibrations and the need for matrix-matched standards. Therefore, XRD can be used to verify or complement the test results of other chemical analysis methods. Parameters such as total iron content or total Fe₂O₃ content can be derived.

The major advantages of XRD are speed and simplicity of the sample preparation. Preparation, measurement, and data evaluation take a few minutes in total. The fine milled powder should have an average particle size of about 10 microns. The powder only needs to be put to a sample holder having a flat and smooth surface.

XRD is complementary and competitive to so-called automated mineralogy surface analytical techniques, such as light microscopy and analytical scanning electron microscopy. Here, the particular strength of XRD is its sensitivity to the fine particle fraction that is hardly accessible to microscopy. Again, XRD sample preparation is quick and simple, whereas surface methods require the time-consuming preparation of polished blocks. Only XRD can distinguish polymorphs (e.g. TiO₂ in the form of rutile or anatase) and polytypes (e.g. Muscovite 1M or 2M1).



XRD can be used to explain severe recovery losses. Yield estimates are typically based on chemical analysis. However, iron may be locked in minerals that are removed during the beneficiation of the ore, or which are inaccessible to the extraction process. Such carrier minerals could be gibbsite or ferrous dolomite (ankerite). Chemical analysis does not know about element speciation, whereas a simple peak position analysis of the XRD data tells the amount of non-extractable iron.

The stepwise loss on ignition (LOI) in thermo-analysis, which is frequently combined with XRF, tells about the amount and type of volatiles, such as CO₂, H₂O, and OH, and is only an indirect measure of the hydroxide and clays mineralogy in iron ore. XRD directly measures these minerals.

Raw iron producers contribute to major greenhouse-gas pollutants. The CO₂ footprint of a pig-iron plant is mainly governed by the overall oxidation state (Fe²⁺/Fe³⁺) of iron in the ore. The oxidation state determines the amount of reducing agent (coal) in raw iron production and is obtained from the mineralogy of the ore. XRD is not only fast but virtually operator independent, especially when compared to wet chemical methods such as titration.

Bruker AXS Inc.
 Madison, WI, USA
 +1 (800) 234-9729
 info@bruker-axs.com
 www.bruker-axs.com