

Chemical trace analysis in materials

Chemical trace analysis of materials plays a crucial role in various industries, from materials science and environmental analysis to the food, pharmaceutical, semiconductor and aerospace industries. This analysis makes it possible to identify and quantify the smallest amounts of chemical substances in materials, which is essential for quality assurance, compliance with regulations and evaluation of material suitability.

Importance of trace analysis in materials

Quality is crucial in the production of materials. Impurities or undesirable chemical residues can have a significant impact on the properties of a material. Trace analysis enables manufacturers to ensure that their products meet the required standards and have the desired properties. In addition, in many applications, especially in the food and pharmaceutical industries, product safety is of paramount importance. The identification of harmful chemicals or residues in materials is crucial to minimize potential health risks. The cleanliness of products also plays a major role for many applications in the high-tech sector, such as the semiconductor and aerospace industries. Contamination can hinder the functionality of the application or reduce the service life of the machines. In materials research, analyzing chemical traces is crucial to developing new materials and understanding their properties. This can lead to innovation in various fields, from nanotechnology to sustainable material development. Not to forget the regulatory requirements, which often demand a detailed analysis of materials to ensure that they do not contain harmful substances. In this case too, chemical trace analysis is essential for companies to demonstrably ensure compliance with regulations.

Insights into some methods of chemical trace analysis

There are a variety of different methods for chemical trace analysis, which are used depending on the area of application and the materials to be analyzed. The most common methods with some advantages and disadvantages are briefly described below.

Gas Chromatography (GC)

Gas chromatography is a widely used method for separating and analyzing volatile compounds. It enables the identification and quantification (in the ppb range) of chemical substances in complex mixtures.

Liquid Chromatography (HPLC)

High-performance liquid chromatography is a method for analyzing non-volatile and thermally unstable compounds. It is frequently used in the pharmaceutical industry to identify and quantify active ingredients and their impurities (in the ppm range).

Mass Spectrometry (MS)

Mass spectrometry is a powerful technique for identifying molecules based on their mass-to-charge ratio. It is often used in combination with chromatography methods to increase the sensitivity and specificity of analyses.

Atomic Absorption Spectrometry (AAS)

Atomic absorption spectrometry is used to quantify metallic elements in materials. This method is particularly useful in environmental analysis and materials science to identify heavy metals and other trace elements (approx. in the ppm range).

X-Ray Fluorescence Analysis (XRF)

X-ray fluorescence analysis is a non-invasive method for determining the chemical composition of materials. It is frequently used in materials testing and the recycling industry to analyze the composition of alloys and other materials. It provides the elemental composition in the bulk of the material (down to approx. 100 μm).

Time-Of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS)

Time-of-flight secondary ion mass spectrometry is a high-resolution mass spectrometry technique that analyzes secondary ions from the surface of a material to determine its chemical composition. This method allows surfaces to be analyzed with a high spatial resolution and is particularly useful for the investigation of thin films and surface modifications. The penetration depth of TOF-SIMS is approx. $< 1 \text{ nm}$.

Energy-Dispersive X-Ray Spectroscopy (EDX)

Energy dispersive X-ray spectroscopy is an analytical technique used in combination with scanning electron microscopy (SEM) to determine the chemical composition of materials by analyzing the characteristic X-rays emitted by the elements. This method provides a fast and effective way of analyzing the elemental distribution in samples (penetration depth approx. $1 \mu\text{m}$) and is particularly useful for analyzing solid materials.

Mass Spectrometry with Inductively Coupled Plasma (ICP-MS)

Inductively coupled plasma mass spectrometry is a highly sensitive analytical method that makes it possible to determine the concentrations of elements in a sample by ionisation in an inductively coupled plasma and subsequent mass spectrometry. This technique is particularly effective for analyzing trace elements in complex matrices and offers high sensitivity (ppt range).

Infrared Spectroscopy (IR)

Infrared spectroscopy is a method for identifying and characterizing chemical compounds by measuring the absorption of infrared light. Molecules absorb specific wavelengths of infrared light, which leads to characteristic vibrations that are visualized as a spectrum and provide information about the molecular structure. Infrared spectroscopy is a fast and inexpensive method, but with very low sensitivity (ppm).

X-Ray Photoelectron Spectroscopy (XPS)

X-ray photoelectron spectroscopy is a method of chemical analysis in which X-rays are used to remove electrons from the inner shells of an atom. The energy of the emitted electrons is measured to obtain information about the chemical composition and the bonding states of the elements on the surface (up to approx. 3 nm) of a material.

Table 1: Selection of some common chemical trace analysis methods

	Equipment costs	Measurable sample composition	Sample preparation effort	Predominant result type
GC	medium	volatile compounds	medium	quantitative
HPLC	medium	liquid	medium	quantitative
MS	medium	solid, liquid, gaseous	high	quantitative
AAS	low	liquid, solid	medium	quantitative
XRF	medium	solid	low	quantitative
TOF-SIMS	high	solid	high	qualitative (semi-quantitative)
EDX	medium	solid	low	qualitative (semi-quantitative)
ICP-MS	high	liquid	high	quantitative
IR	low	solid, liquid	low	qualitative (semi-quantitative)
XPS	high	solid	high	quantitative

Suppose a company develops an innovative, high-performance polymeric material specifically designed to meet the demanding requirements of the aerospace industry. To ensure that this material meets all the required specifications, it is essential to precisely analyze the composition of the elements and assess the state of cleanliness. Choosing the right chemical trace analysis method can be crucial here.

An experienced specialist can help to select the optimal analysis method. For example, time-of-flight secondary ion mass spectrometry (TOF-SIMS) could be recommended to precisely analyze the surface composition and distribution of elements in the polymer. Alternatively, energy dispersive X-ray spectroscopy (EDX) could be used to determine the elemental composition and distribution within the material. Fourier transform infrared spectroscopy (FTIR) could also be used to analyze the chemical bonding states and functional groups in the polymer. The expertise of a specialist ensures that the chosen method meets the specific requirements and issues of material development and delivers precise, reliable results. This not only saves time and resources, but also significantly increases the project's chances of success.

In view of the large number of different chemical analysis methods, it can be a challenge to find the right method for the problem at hand. At Materiales GmbH, we have state-of-the-art technologies, specialized expertise, and an extensive network of reliable laboratory service providers. This enables us to offer you customized solutions that are precisely designed to your specific needs and requirements. Benefit from our many years of experience and our wide range of analysis methods. Contact us to find out more.