



ToF-SIMS

Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) is an analytical method for the chemical characterisation of solid surfaces. With this method, the atomic and molecular composition of the outermost 1-3 monolayers is obtained. ToF-SIMS can be used on conducting and insulating surfaces. With detection limits in the ppm range also small amounts of a compound can be probed with high sensitivity.

SIMS analysis is based on a simple principle. The surface under study is bombarded with a primary ion beam of high energy (e.g. Au⁺ or Bi⁺). The projectile's energy is transferred to the region near the surface by collisions between the primary ions and the sample atoms as well as by collisions between sample atoms. This collision cascade transports a small part of the energy back to the surface and leads there to emission of electrons, neutrals and secondary ions (= sputtering; see fig. 1). Subsequently, the secondary ions are analysed with respect to their mass to charge ratio in a suited analyser.

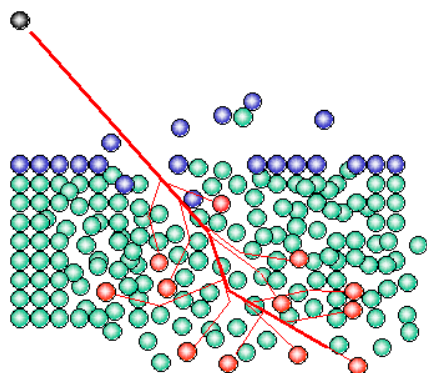


Figure 1: Schematic of the excitation processes in SIMS (Collision cascade; grey: primary ion; blue: atoms from the outermost monolayers; green: atoms in deeper layers; red: sample atoms after a direct collision with the primary ion).

In ToF-SIMS the mass of the sputtered secondary ions is determined by means of a Time-of-Flight (short: ToF) mass analyser. For the mass analysis all secondary ions which were produced by a short primary ion pulse are accelerated to the same energy. From the time

needed to travel along a given drift path the mass of each secondary ion can be calculated. In this way, an accurate determination of the flight time yields the chemical composition of the emitted ions and thus the elemental and molecular composition of the sample surface. In modern analysers this parallel mass detection is combined with an excellent capability to separate masses that are closely together (e.g. Fe⁺ (55,9349u) and Si₂⁺ (55,9539u)).

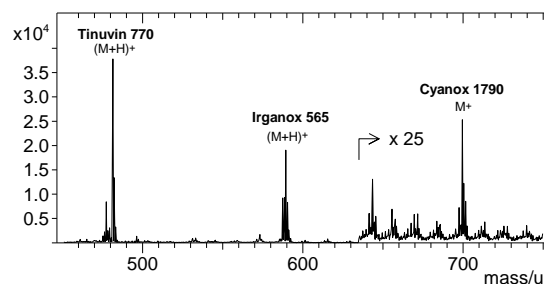


Figure 2: Positive secondary ion spectrum of polymer additives in Low Density Polyethylene (LDPE).

The intensity of the detected secondary ions is influenced by the chemical composition of the surrounding matrix material (SIMS matrix effect). Therefore, SIMS does not give inherently quantitative data. However, it is possible to compare analyses of chemically similar samples. Furthermore, with the analysis of suitable references it is possible to determine absolute concentrations.

The sample bombardment with primary ions leads to changes in the local molecular structures. Therefore only very few primary ions can be used for the determination of the original composition of the surface (Static SIMS, spectrometry). The resulting spectra are records of the intensity as a function of the mass of the secondary ion and represent the average composition of the probed area (see fig. 2).

The chemical distribution can be recorded as an image by scanning the area pixel by pixel with a focussed primary ion beam (imaging or mapping, see fig.3). The intensity in each pixel



is assigned a colour value, leading to mass resolved images. The size of the analysed surface can be varied from about $20 \times 20 \mu\text{m}^2$ to $500 \times 500 \mu\text{m}^2$. Larger areas of up to $9 \times 9 \text{cm}^2$ can be addressed by automated movement of the sample during the analysis (stage scan). The in routine operation attainable minimum diameter of the primary ion beam is approximately 300 nm.

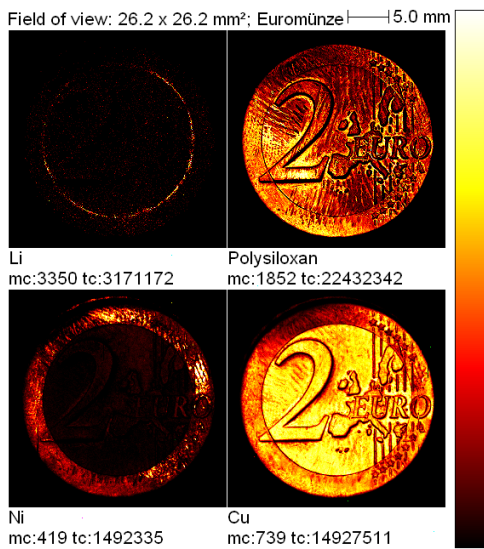


Figure 3: Selected secondary ion images of a 2 euro coin (mc: number of secondary ions in the brightest pixel; tc: total counts of detected secondary ions). The detected polysiloxane is a component of hand lotions, among others.

The damaging effect of the primary ion bombardment can be utilised if one wants to investigate the chemical build up of a sample as a function of depth. By applying high ion doses so-called depth profiles can be generated. Depending on the chosen bombardment conditions profiles can be performed for elemental (e.g. metallic layers) as well as organic (e.g. organic light emitting diodes (OLED)) layer sequences. During the analysis the chemical composition of the crater bottom is acquired as function of sputter dose or time. Depth scales can be established at the end of an analysis when the final crater depth is determined or if a sputter yield of the matrix material is known (see fig. 4).

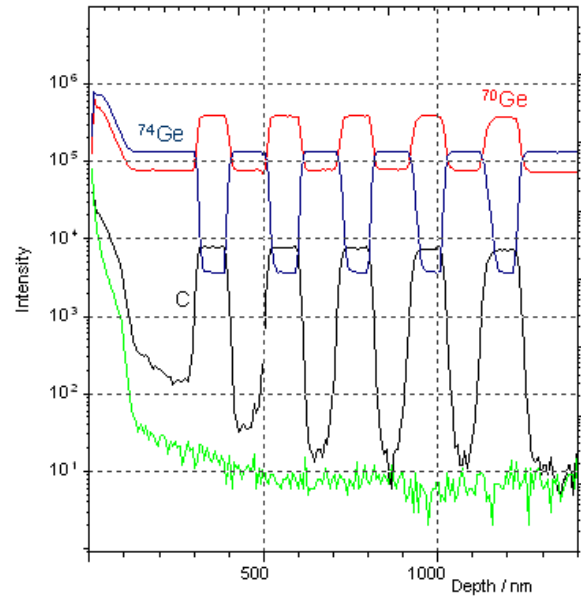


Figure 4: Depth profile for a Ge multi layer system; (Source: Prof. Bracht; Inst. für Materialphysik, WWU Münster)

The combination of imaging and depth profiling yields a "3D-analysis" mode of operation (see fig. 5). This makes it possible to probe a complete sample volume with good resolution in all 3 dimensions and serves among others in the identification of point defects in complex layer structures.

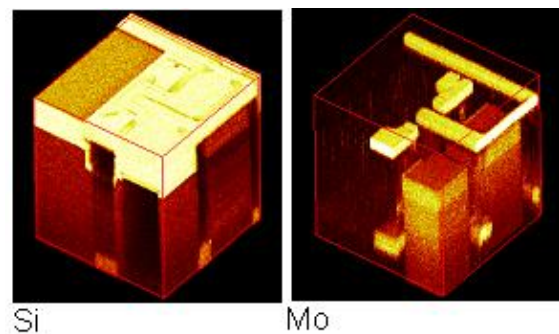


Figure 5: 3D-image for the Si and Mo distribution in a pixel from a TFT monitor.