ABSTRACT

Secondary ion mass spectrometry (SIMS) is an analytical experimental technique, used for compositional analysis of solid surfaces and thin films. When a surface is bombarded by high energy beam of primary ions, secondary particles are emitted. Few of them are charged ions (secondary ions), which are detected and analysed by a mass spectrometer. Depending on the operating mode selected, SIMS can be used for surface composition and detailed chemical structure analysis, depth profiling or imaging of complex solid surfaces and thin films to a depth of 1 to 2 nm. Due to its low detection limits and high surface sensitivity it gives us information complementary to other spectroscopic techniques. This seminar reviews the basic principles, instrumentation and a typical application used in SIMS.
Secondary ion mass spectrometry (SIMS) is an analytical method with very low detection limits. It is capable of analysing over a broad dynamic range, has high surface and chemical sensitivity and high mass resolution [1]. In this technique, primary ions (ion clusters) are used to sputter a thin film or solid surface of any composition. This causes the emission of secondary particles: atoms, electrons, ions and neutral species from the target. A pictorial representation of the process is shown in Figure 1.

The most of emitted particles are neutral (99%) and lost for detection [2]. Some of emitted particles are ionized (1%) in the course of leaving the surface. Those ions, so called secondary ions, are accelerated with high voltage (range of kV) towards mass spectrometer, where they are sorted depending on their mass to charge ratios. From mass spectrum we can determine type of secondary ions and identify molecular structure of the surface. SIMS method can be compared with other surface and chemical sensitive methods like scanning electron microscopy (SEM), which is usually used in combination with energy dispersive X-ray spectroscopy (SEM/EDXS) in energy range between 0 and 10 keV. SEM/EDXS combines scanning of electron beam of energy of 10 - 30 keV with high lateral resolution and gives information about elemental composition (C, O, Fe,…). The SIMS method also combines scanning with information about chemical structure ($C_xH_yO_z$, Al-
OH, H,...). SIMS method has much higher surface sensitivity (1 nm) whereas the “surface” sensitivity of EDXS is about 1 µm. The use of each of them depends on specific application.

2. BASIC CONCEPTS

2.1 Ion sputtering

Bombarding surface with focused beam of high energetic ions (10 - 40 keV) causes particle ejection from the surface [2]. This process is known as ion sputtering. Sputtering occurs as the result of a series of elastic and inelastic collisions. By elastic collisions momentum is transferred from the incident particles to the target atoms, causing other collisions to occur within the target [3]. Eventually, a target atom is ejected from the surface as a sputtered particle, if it receives a component of kinetic energy that is sufficient to overcome the surface binding energy of the target material. Some of the ejected atoms may be ionized. Inelastic interactions are shown as the production of photons or emission of secondary electrons and vibrations of crystal lattice released with local warming of the target.

When a solid material is sputtered with an ion beam, a number of mechanisms operate to slow the ion and dissipate the energy [4]. Interactions inside the target and types of secondary processes by ion sputtering are shown in Figure 2.

![Figure 2: Interaction of impact ion with the surface: (1) Impact ion hits the surface/target. (2) Ion reflection. (3) Ion implantation. (4) Secondary electron emission. (5) Surface damage and atom migration. (6) Structural changes of target. (7) Ion energy gets lost in the target. (8) Sputtered atom or ion (ion sputtering). (9) Local warming of the target. [4]](image)

(1) High energy particle hits the surface.
(2) Impact ion is reflected from the surface.
(3) If impact ion is not backscattered out of the target surface, it will eventually come to rest, implanted within the target at some depth below the specimen surface. This phenomena is known as ion implantation.
(4) Collision of ion to the surface can cause emission of one ore more secondary electrons from the target.
(5) Ion can cause changes in target structure by changing atom positions. Atom can occupy interstitial place in crystal structure, on the old spot the blank is left. Radiation damages can occur (ion beam mixing).
(6) Ion can cause series collisions between atoms of target that leads to change of its composition and structure.
(7) Collision energy can get lost in the target.
(8) Impact ion can cause ejection of one or more atoms from the target surface. This desorption (sputtering, erosion) atoms or ions from the solid surface, as a consequence of
ion bombarding, is known as ion sputtering. Sometimes group of atoms (molecules) are sputtered from the surface. This is a main event followed by the SIMS technique.

(9) Local warming of the target, which leads to higher atom migration.

Particles, sputtered from the surface of solids, are emitted with a range of kinetic energies [3]. The kinetic energy distribution is influenced indirectly by the primary ion energy (E₀), angle of incidence and structure, which will determine the nature of the collision cascades in the material. With each collision, the incident ion losses energy and changes direction by an angle φ. Using conservation of momentum, the recoil energy of struck atom (M₁) is transferred to target atom (M₂). Energy T, transferred to target atom can be written as:

\[ T = \frac{4M₁M₂}{(M₁ + M₂)^2} E₀ \sin^2 \frac{\phi}{2} \]  

(1)

The energy, deposited by an ion is distributed in electronic excitations and kinetic energy that ends up in atomic motion and damage. The key quantity in energy loss considerations is the stopping force dE/dx [5]. It can be considered as the force that the medium exerts on the penetrating particle:

\[ \frac{dE}{dx} = NS(E) \]  

(2)

where N is the number density of atoms in the medium and S(E) the stopping cross-section, which is the average energy transferred when summed over all impact parameters. Ion range (R) is defined as the integrated distance that an ion travels while moving in a solid and is inverse related to stopping force:

\[ R = \int_0^\infty \frac{dE}{\frac{dE}{dx}} = \int_0^\infty \frac{dE}{NS(E)} \]  

(3)

Impact between primary ions and the surface atoms can be divided into collisions between the primary particle and the nuclei, and those between the primary ion and the electrons. The first type of collisions occurs for small impact parameters and lead to a large-angle scattering process, whereas the latter ones lead to energy loss without any significant deflection of the primary particle. The stopping cross-section S(E) can be split up into

\[ S(E) = S_n(E) + S_e(E) \]  

(4)

where \( S_n \) is the nuclear stopping cross-section and \( S_e \) the electronic stopping cross-section. The nuclear stopping is dominant by lower energies (E ~ keV), but decreases gradually for higher energies (E ~ MeV), where electronic stopping is present. The nuclear stopping for all target–beam combinations could be expressed as

\[ NS_n(E) = \frac{\pi a_l^2 \gamma N}{(E/E)} S_n(e) \]  

(5)

where \( \gamma = 4M_1M_2/(M_1 + M_2)^2 \)  

(6)

is determined by the maximum energy transfer from a particle of mass M₁ with an energy E to a particle at rest with mass M₂ and by Lindhard’s screening parameter

\[ a_L = 0.8853a_B \left( Z_1^{2/3} + Z_2^{2/3} \right)^{-1/2} \]  

(7)

An important scaling parameter is Lindhard’s reduced energy ε
The absolute magnitude is determined partly by the factor \((\varepsilon/E)\) in the denominator, which means that for heavy atoms on a heavy target the factor becomes small and, in turn, leads to a large nuclear stopping. Equation (6) also demonstrates that \(\varepsilon\) decreases with increasing atomic number (and mass) of the projectile. The electronic stopping \(S_e\) for the high energy ions can be expressed as

\[
S_e(E) = \frac{4\pi Z_1^2 Z_2 e^4}{m_v^2} \ln \left( \frac{2m_v^2}{I} \right)
\]

where \(v\) is ion velocity and \(I\) the mean ionization potential. Proportion between number of sputtered atoms divided with number of incident ions is known as sputtering yield (Y) [3]. It increases with primary particle mass and energy. It depends on type of target atom, binding energy of target atoms, angle of incidence. For lower energies it can be written as:

\[
Y = \frac{3\alpha}{4\pi^2} \frac{4M_1 M_2}{M_1 + M_2} \frac{E}{U_0}
\]

where \(U_0\) is the surface binding energy, parameter \(\alpha\) depends on ratio \(M_2/M_1\). Y tends to maximize by energy 5 - 50 keV [2]. Beyond this energy yield drops away as the primary beam penetrates deeper into the solid and less energy returns to the surface region. Generally the larger the mass of the bombarding particle, the closer to the surface the energy will be deposited and greater will be the yield. Since larger ions have been shown to deliver significantly higher ion yields, there has been increasing interest in the use of polyatomic cluster primary ions. First instruments used atomic ions (Ar\(^+\), Cs\(^+\), Ga\(^+\)) for the primary beam ions, in recent years ionized molecules (SF\(_5^+\)), ionized clusters of gold and bismuth (Au\(_{n}^+\), Bi\(_n^+\)), large gas cluster ion beams (Ar\(_{2500}^+\)) or fullerene (C\(_{60}^+\)) have come in use. In Figure 3 the sputter yields of water molecules from ice under Au\(_{n}^+\) and C\(_{60}^+\) bombardment are compared. There is a dramatic increase in yield between the atomic projectile Au\(^+\) and the cluster ions of Au\(^+\)_n. The cluster breaks up as it hits the surface and the projectile energy is portioned between all the atoms. Due to larger size they penetrate the material much less and generate less chemical damage [5]. Sputtering yield depends on the strength of chemical bonds, but it does not depend on crystal structure. Because of shallower implantation depth and higher sputtering yields cluster ions are very suitable for molecular depth profiling of most organic and biological samples, where in-depth molecular distribution is measured.

<table>
<thead>
<tr>
<th>Removed # of H(_2)O Equivalents</th>
<th>100</th>
<th>575</th>
<th>1190</th>
<th>2510</th>
</tr>
</thead>
<tbody>
<tr>
<td>Au(^+)</td>
<td>Au(_2^+)</td>
<td>Au(_3^+)</td>
<td>C(_{60}^+)</td>
<td></td>
</tr>
</tbody>
</table>

**Figure 3**: Sputter yields of water molecules from ice under bombardment by 20 keV Au\(^+\)_n ions compared with C\(_{60}^+\) clusters [2].
2.2 Ionization

The secondary process (ionization) occurs by the emission of particles from the surface, inside or outside the target [1]. By ionization outside the target sputtered particle relaxes by emitting an Auger electron, thus becoming an ion. Ionization inside the target is described by the bond-breaking model, where the primary particle causes heterolytic cleavage of a bond in the target. Either an anion or a cation is emitted directly from the target surface. The yield of secondary ions is strongly influenced by the electronic state of the material being analysed (matrix effect). In SIMS, matrix effects are common and originate from changes in the ionisation efficiency and the sputtering yield. One of the main causes of matrix effect is the primary beam. Electronegative primary ions increases the number of positively charged secondary ions, while electropositive primary ions increase the number of negatively charged secondary ions. Matrix effect can also be caused by species present in the sample and the composition of the sample.

For organic materials, the mechanism of secondary ion formation is far from fully understood. Primary high energy ion impact on organic material (thin film) causes emission of atomic species and the fragmentation of the organic backbone. In the case of covalent molecular solids with directed bonds, energy is transferred through vibrations. In polymeric material the primary particle induces a physical scission in the polymer chain, which yields a macro-radical or ion. As the primary ion energy is transformed into vibrational energy within the bonds of the molecule, the polymer is unzipped from the point of fragmentation and successively larger lower energy fragments are emitted. Internal excitation leads to fragmentation via chemically determined pathways. Atomic species and small uncharacteristic organic fragments are thought to be emitted directly from the point of primary ion impact. Sputtering of metal substrate leads to collision cascades in the material. The energy, initially deposited by the primary particle falls off exponentially with successive collisions of recoiling atoms, transferring decreasing amounts of energy to adsorbed molecules. Since the kinetic energy of the atoms set in motion is much larger than the binding energy of the material, the standard treatment for metals can be largely extended to semiconductors and insulators [7].

In general, desorption of secondary ions after bombardment the surface with primary ions does not depend on crystal structure, but more on the type of chemical bonds, i.e. on local chemical environment. The ionization probability of secondary ions, which are of the main interest in SIMS, depends very strongly on type of other atoms and species present on the surface since they can contribute to a charge transfer from desorbed particle and thus increase or decrease the SIMS signal.

3. EXPERIMENTAL REQUIREMENTS

The fundamentals in SIMS were laid by Herzog and Viehboeck in 1949, in 1950 Honig constructed the first complete SIMS spectrometer capable of sputter depth profiling [2]. In SIMS spectrometer there are three main components: the primary particle source, mass analyser and detector. During measurement an ultra high vacuum with pressure below $10^{-6}$ mbar is required. It prevents collision of secondary ions with background gases on their way to the detector and surface contamination by adsorption of background particles. The basic arrangement for the SIMS experiment is shown in Figure 4.
3.1 Primary particle source

Primary particles for the sputtering process can be supplied in a number of ways: by plasma, an ion source, an accelerator or by a radioactive material emitting alpha particles [2]. From the construction point of view there are three basic types of ion guns [6]. In one, ions of gaseous elements are usually generated by electron ionisation, for instance noble gasses ($^{40}$Ar$^+$, Xe$^+$), oxygen ($^{16}$O$^-$, $^{16}$O$_2^-$, $^{16}$O$_3^-$), or ionized molecules (SF$_5^+$, C$_{60}^+$). This type of ion gun is easy to operate and generates roughly focused but high current ion beams. A second source type, the surface ionisation source, generates $^{133}$Cs$^+$ primary ions. Cesium atoms vaporize through a porous tungsten plug and are ionized during evaporation. Depending on the gun design, fine focus or high current can be obtained. A third source type, the liquid metal gun (LMIG), operates with metals or metallic alloys, which are liquid at room temperature or slightly above. The liquid metal covers a tungsten tip and emits ions under influence of an intense electric field. LMIG provides a tightly focused ion beam (<60 nm) with moderate intensity. Because of it’s ability to generate short pulsed ion beams it is commonly used in static Tof SIMS instruments, described in next chapter.

The choice of the ion species and ion gun respectively depends on the required current (pulsed or continuous), required primary beam dimensions and on the sample which is to be analysed [1]. Oxygen primary ions are often used to investigate electropositive elements due to an increase of the generation probability of positive secondary ions, while caesium primary ions often are used when electronegative elements are being investigated. For short pulsed ion beams in static SIMS, LMIGs are most often deployed for analysis; they can be combined with either an oxygen gun (E= 1 - 3 keV) or a cesium gun (E=1 - 3 keV) during elemental depth profiling, or with a C$_{60}^+$ (E= 20 - 30 keV, 500 eV per C atom) or gas cluster ion source (E= 20 - 30 keV) during molecular depth profiling.

3.2 Primary ion column

Primary ion column is an optical system with function of accelerating and focusing the beam onto the sample and separating the primary ion species by Wien filter or pulsing the beam (in Tof-SIMS) [2]. Wien filter is a device consisting of perpendicular electric ($E$) and magnetic ($B$) fields that can be used as a velocity filter for charged particles. When ion velocity ($u$) does not equal proportion $E/B$, the trajectory curves up or down, as shown in Figure 5.
For ions with velocity $u$ proportion of mass and ion charge ($m/Z_o$) can be written as

$$m/Z_o = 2V(B/E)^2,$$

where $V$ is accelerating potential of primary ions. With Wien filter we assure selection of primary ions depending on proportion of mass and ion charge based on this equation.

### 3.3 Mass analyser

Depending on the SIMS type, there are three basic analyzers available: sector, quadrupole, and time-of-flight [6]. They differ with respect to transmission, mass resolution, mass detection (parallel or sequential) and sensitivity. A **sector field mass spectrometer** uses a combination of an electrostatic and a magnetic analyzer to separate the secondary ions by their mass to charge ratio [2]. Ions are extracted from the sample using a high extraction potential. Upon traversing a magnetic field, a charged particle experiences a field force in a direction orthogonal to the direction of magnetic flux lines and its original axis of travel. It adopts a circular path. The extent of force experienced by the particle and hence the radius of its path is directly related to its velocity. Since all ions are accelerated to a fixed potential before entering the magnetic field they can be readily separated according to their masses.

The radius of curvature $R$ for an ion of mass to charge ratio $m/Z_o$ traveling through a magnetic field $B$ having been accelerated by potential $V$ is given by:

$$R = \frac{1}{B}(2mV/Z_o)^{1/2}$$

The dispersion of adjacent masses (mass resolution) is proportional to the radius of the magnets used and degrades with increasing mass. A **quadruple mass analyser** separates the masses by resonant electric fields, which allow only the selected masses to pass through. It makes use of a combination of a DC and a radio frequency electric field applied to four parallel rods, in order to separate ions according to their mass to charge ratio. A potential consisting of a constant DC ($U$) component plus an oscillating RF component ($V \cos \omega t$) is applied to one pair of rods whilst an equal but opposite voltage is applied to the other pair. The rapid periodic switching of the field sends most ions into unstable oscillations of increasing amplitude until they strike the rods and are hence not transmitted. Ions with a certain $m/Z_o$ follow a stable periodic trajectory of limited amplitude and are transmitted to the detector. By increasing the DC and AC fields whilst keeping a constant ratio between them, this resonant condition is satisfied for ions of each ascending $m/Z_o$ ratio in turn. The **time of flight mass analyser** separates the ions in a field-free drift path by their velocities. Since all ions possess the same kinetic energy the velocity and therefore time of flight varies according to mass. According to the equation of kinetic energy, heavier masses
travel more slowly. The measured flight time $t$ of ions of $m/Z_0$, accelerated by a potential $V$ down a flight path of length $L$ can be written as

$$t = L(m/2VZo)^{1/2}$$  \hspace{1cm} (13)

It requires pulsed secondary ion generation using either a pulsed primary ion gun or a pulsed secondary ion extraction. It is the only analyzer type able to detect all generated secondary ions simultaneously, and is the standard analyzer for static SIMS instruments.

3.4 Detectors

Most modern mass spectrometers have more than one detector: an electron multiplier, a Faraday cup, an image plate detector and a resistive anode encoder [7]. Only one detector can be used at any time. Signal from detectors is multiplied, transmitted to digital form and analysed with specific computer programs. The electron multiplier is the most sensitive detector. It must be protected from intense ion beams (>5x10^6 c/s) as these can rapidly lead to its destruction. It consists of a series of electrodes called dynodes. Each dynode is connected to a resistor chain. The first dynode is at ground potential, so that both positive or negative ions may be detected. When a particle (ion) strikes the first dynode it may produce a few (1 - 3) secondary electrons. These secondary electrons are accelerated to the second dynode that is held at a slightly higher positive potential. On impact more secondary electrons are generated and a cascade of secondary electrons ensues. A Faraday cup detector can detect count rates from 5x10^4 c/s upwards. It does not discriminate between the type of ion or its energy. It is simple and cheap, but its response time is slow. It consists of a hollow conducting electrode connected to ground via a high resistance. The ions hitting the collector cause a flow of electrons from ground through the resistor. The resulting potential drop across the resistor is amplified. An ion image plate consists of an array of miniature electron multipliers (channels) composed of lead glass. An ion passing down a channel hits the inner channel wall and produces secondary electrons. The channels are designed so that these secondary electrons initiate an electron cascade down the channel. The pulse of electrons from the back of the detector may either be passed to a second micro channel plate for further gain, or accelerated towards a phosphor screen, where their impact may be viewed directly. The resistive anode encoder is a position-sensitive detector, used to digitally record ion images. It uses a micro-channel plate for the ion to electron conversion, so it discriminates between species. An ion entering a channel in the first of two micro-channel plates. The ion to electron conversion results in a pulse of electrons that emerge from the back of the first plate to initiate a second electron cascade in the channels of a second plate. The resulting electron pulse strikes a resistive plate comprising a thick resistive film, deposited on a ceramic plate. The charge pulse is partitioned off to four electrodes at the corners of the plate.

4. OPERATION MODES

Ideally, any analytical measurement should not change the structure of sample being measured. Surface or structure damage may lead to incorrect results of analysis, so it is important to keep the current density low and the sampling time as short as possible. Since during the SIMS analysis the surface atoms are removed from the surface, SIMS is...
locally destructive technique [6]. Emitted particles originate from the 1–2 monolayers (depth of 1 nm), so it is also a surface sensitive technique. In order to obtain chemical information of the original surface, the primary ion dose must be low enough to prevent a surface damage. This regime is so-called "static SIMS" mode and it is widely used for the characterization of polymer surfaces - atomic monolayer analysis or surface molecular analysis, usually with a pulsed ion beam and a time of flight mass spectrometer. If the primary ion dose is large enough it can be used to erode the surface layer in a controlled manner (sputtering process). In this way information on the in-depth distribution of elements can be obtained. This, so called "dynamic SIMS" mode is widely applied for depth-profiling of thin films, layer structures and dopant concentration, using a DC primary ion beam and a magnetic sector or quadrupole mass spectrometer. Layers of up to few microns thick can be depth-profiled using SIMS technique. In principle, combining one of the mass analyser systems with a liquid metal ion source enables surface analysis with high spatial resolution to be carried out [2]. This process is known as “SIMS imaging”. Highly focused ion beam (beam diameter of 50 nm) is digitally rastered over the surface of interest from point to point like in scanning electron microscope (128 x 128 pixels). At each pixel point it is possible either to collect ions of a single \( m/z \), of a few specified \( m/z \) or a whole mass spectrum (typical mass region 0 - 1000 u), dependent on the detail required and the sophistication of the analyser and data system. After imaging of an area (10 x 10 - 200 x 200 \( \mu m^2 \)) different chemical images can be constructed from signals at different masses. In this way a lateral distribution of molecules of particular mass (for example H, C\( x \)H\( y \)O\( z \), Si-O) can be obtained. Lateral resolution in SIMS imaging mode is determined by diameter of the ion beam and it is typically from 50 - 100 nm. For comparison, the lateral resolution in SEM method is about 1nm and SEM/EDXS imaging is 1 \( \mu m \) since it is determined by region of X-ray generation. The example of SIMS image is shown in Figure 6.

Figure 6: TOF-SIMS images obtained on the cotton fibers treated with fluoroalkylsilane. Images on left side were obtained summarizing the signals of Si\( x \)O\( y \) clusters (left top), fluorocarbon (left middle) and aliphatic hydrocarbons (left down). An image on the right side is a composite image obtained from three images on the left. The primary ion was 25 keV Bi\( 3^+ \). The peaks from positive SIMS spectra were selected for images. Lateral resolution in this case was about 100 nm. [6]

5. APPLICATION

In SIMS analysis the spectra of positive and negative ions are measured [6]. Whole mass spectrum is acquired at very high sensitivity level (ppm). The typical acquisition of SIMS spectrum at one point takes about 1 - 3 min. It depends on the required mass region (typically 0 - 1000 u) and mass resolution (typically \( m/dm \sim 5000 \)). This time is shorter
than typical time needed for acquisition of high-energy resolution spectra of different elements in other analytical techniques (XPS analysis). In the following an example of application of static SIMS technique for surface characterization of polymer PET (C_{10}O_{4}H_{8})_n is given. Its structural formula is shown in Figure 7.

![Structural formula of polymer PET.](image)

**Figure 7:** Structural formula of polymer PET.

Analysis was performed in the SIMS spectrometer produced by ION TOF company, model “TOF.SIMS 5”, which was recently installed at Department of Surface Engineering and Optoelectronics at Jozef Stefan Institute. During the analysis polymer samples are usually charging electrically so a low-energy electron gun-neutraliser (5 eV) was used. The analysis took place in an ultra-high vacuum (10^{-9} mbar), the time-of-flight mass analyzer was used. Primary ion beam of bismuth cluster ions Bi_{3}^{+} with energy 30 keV was produced by LMIG source. A typical SIMS mass spectrum in the range between 1 u and 200 u, obtained for positive and negative ions for polymer PET with assigned peaks is presented in Figures 8 and 9.

![Negative SIMS mass spectrum with assigned peaks of polymer PET.](image)

**Figure 8:** Negative SIMS mass spectrum with assigned peaks of polymer PET. The SIMS analysis was made at Jozef Stefan Institute, research department F4 (Surface Engineering and Optoelectronics).

![Positive SIMS mass spectrum with assigned peaks of polymer PET.](image)

**Figure 9:** Positive SIMS mass spectrum with assigned peaks of polymer PET.
As shown in Figures 8 and 9, spectrum consists of great number of peaks at different masses. Peak assignment is based on the information from library data base about peaks at characteristic masses belonging to expected chemical molecules and their fragments. In SIMS spectra of polymer PET the ions consisting of end groups, fractions of repeat units, or side chains (C<sub>x</sub>H<sub>y</sub>−/+ ) are detected. Negative SIMS spectrum shows the largest concentration of hydrogen ions (H<sup>-</sup>) at mass 1 u, that originates from bonding of carbon and hydrogen atoms (C-H). Other main peaks are present at masses u 12 (C<sup>-</sup>), 13 (CH<sup>-</sup>), 16 (O<sup>-</sup>), 17 (OH<sup>-</sup>), 41 (C<sub>2</sub>OH<sup>-</sup>), 65 (C<sub>5</sub>H<sub>5</sub>−), 120 (C<sub>7</sub>H<sub>4</sub>O<sub>2</sub>−) …, which originate from the C-C/ C-H, C-O, C=O or O=C-O bonding. Positive SIMS spectrum shows the largest concentration of (C<sub>3</sub>H<sub>5</sub>+) ions at 41 u. Other main peaks are present at masses 28 u (C<sub>2</sub>H<sub>4</sub>−), 29 u (C<sub>2</sub>H<sub>5</sub>−), 39 u (C<sub>3</sub>H<sub>3</sub>−), 51 u (C<sub>4</sub>H<sub>3</sub>−), 104 (C<sub>7</sub>H<sub>4</sub>O<sup>+</sup>), 149 (C<sub>9</sub>H<sub>9</sub>O<sub>2</sub>−), 193 (C<sub>10</sub>H<sub>9</sub>O<sub>4</sub>−) … Beside mentioned peaks which were used to identify the molecular structure of the surface, other peaks exist in the positive SIMS spectrum, as for example at 23 u (Na<sup>+</sup>), 28 u (Si<sup>+</sup>), 40 u (Ca<sup>+</sup>), 41 u (CaH<sup>+</sup>). Observation of these peaks is consequence of a very high sensitivity of SIMS method for electropositive elements.

6. CONCLUSIONS

All spectroscopic techniques have their own special capabilities and challenges. The main features of the SIMS technique are the ability to obtain the chemical information of the type of atoms, clusters and molecules at the surface with very high lateral resolution. Similar information can be obtained with SEM/EDXS method, where high lateral resolution imaging is combined with elemental mapping. In comparison to other surface analytical techniques the SIMS offers several advantages, namely the ability to identify all elements, including H and He and the ability to identify elements present in very low concentration levels (ppm). The SIMS technique was used to follow the surface composition, chemical bonds of surface atoms, molecular structures and spatial distribution of polymer PET.

7. BIBLIOGRAPHY

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