Mass spectrometry (MS) and Secondary Ion Mass Spectrometry (SIMS)

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http://img.directindustry.com/images_di/photo-g/tof-secondary-ion-mass-spectrometer-tof-sims-395525.jpg

Goal of the Presentation

- Our main goal is to give some information to the audience about Mass Spectroscopy and Secondary Ion Mass Spectroscopy by discussing their applications, history,advantages,disadvantages and how they work.

What is mass spectrometry (MS)?

http://202.54.226.233/jsp/images/instrument/Mass%20spectrometry.jpg

- Mass spectrometry is an analytical tool used for measuring the molecular mass of a sample.

- For large samples such as biomolecules, molecular masses can be measured to within an accuracy of 0.01% of the total molecular mass of the sample.

- For small organic molecules the molecular mass can be measured to within an accuracy of 5 ppm or less

Structural information can be generated using certain types of mass spectrometers, usually those with multiple analysers which are known as tandem mass spectrometers.

http://www.proteomesoftware.com/images/PNNL%20FTIRC%20MS.jpg

Where are mass spectrometers used?

- Mass spectrometers are used in industry and academia for both routine and research purposes. The following list is just a brief summary of the major mass spectrometric applications.

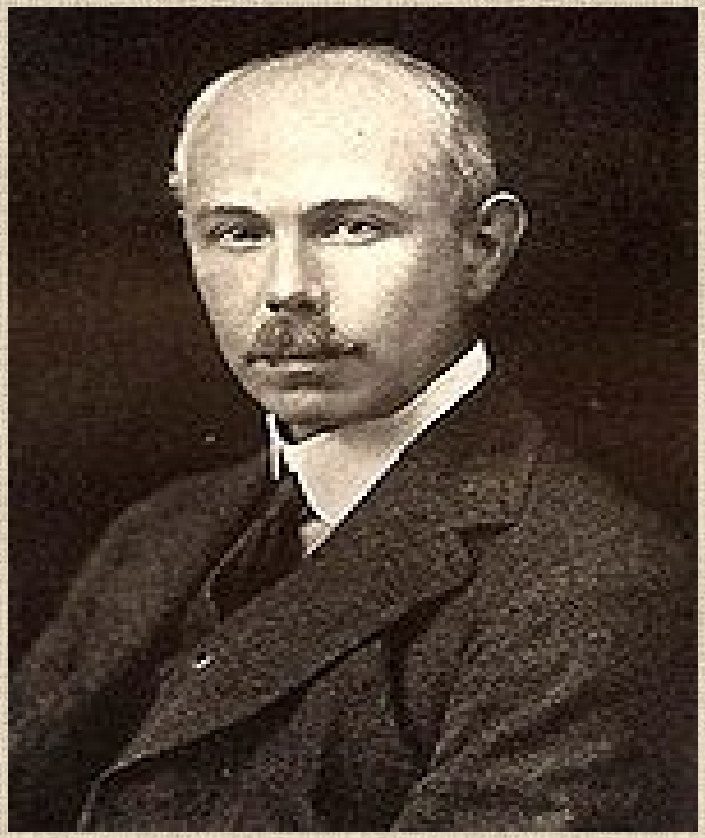
- **Biotechnology:** *the analysis of proteins, peptides, oligonucleotides*
- **Pharmaceutical:** *drug discovery, combinatorial chemistry, pharmacokinetics, drug metabolism*
- **Clinical:** *neonatal screening, haemoglobin analysis, drug testing*
- **Environmental:** *PAHs, PCBs, water quality, food contamination*
- **Geological:** *oil composition*

What is secondary ion mass spectrometry (SIMS)?

http://en.wikipedia.org/wiki/Secondary_ion_mass_spectrometry

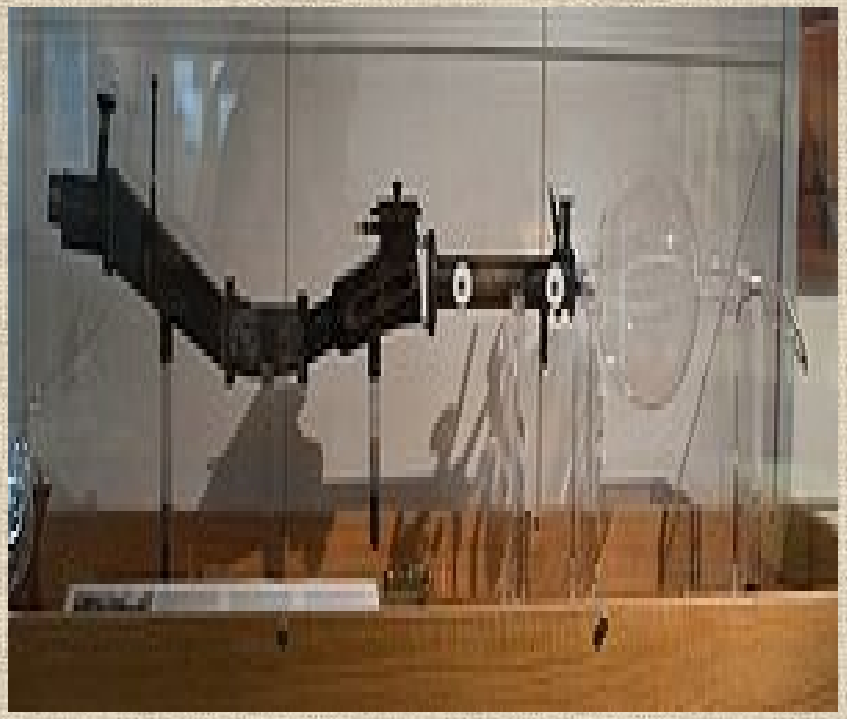
- Secondary ion mass spectrometry (SIMS) is a technique used in materials science and surface science to analyze the composition of solid surfaces and thin films by sputtering the surface of the specimen with a focused primary ion beam and collecting and analyzing ejected secondary ions.
- These secondary ions are measured with a mass spectrometer to determine the elemental, isotopic, or molecular composition of the surface.

History of mass spectrometry



Francis William Aston won the 1922 Nobel Prize in Chemistry for his work in mass spectrometry

- In 1886, Eugen Goldstein observed rays in gas discharges under low pressure.
- Wilhelm Wien found that strong electric or magnetic fields deflected the canal rays and, in 1899, constructed a device with parallel electric and magnetic fields that separated the positive rays according to their charge-to-mass
- The first application of mass spectrometry to the analysis of amino acids and peptides was reported in 1958ratio (*Q/m*).



Replica of an early mass spectrometer

- Some of the modern techniques of mass spectrometry were devised by Arthur Jeffrey Dempster and F.W. Aston in 1918 and 1919 .

- In 1989, half of the Nobel Prize in Physics was awarded to Hans Dehmelt and Wolfgang Paul for the development of the ion trap technique.

History of SIMS

Sir Joseph John Thomson

- In 1910 British physicist J. J. Thomson observed a release of positive ions and neutral atoms from a solid surface induced by ion bombardment.
- Improved vacuum pump technology in the 1940s enabled the first prototype experiments on SIMS at the University of Vienna, Austria.

- In the early 1960s two SIMS instruments were developed. One was an American project for analyzing moon rocks the other at the University of Paris.
- These first instruments were based on a magnetic double focusing sector field mass spectrometer and used argon for the primary beam ions.
- Recent developments are focusing on novel primary ion species like C_{60} or ionized clusters of gold and bismuth.

How mass spectrometer works

If something is moving and
you subject it to a sideways force,
instead of moving in a straight line,
it will move in a curve

Main parts of mass spectrometer

1. Sample input system,
2. İon source,
3. Mass analyser,
4. Detector,
5. Display

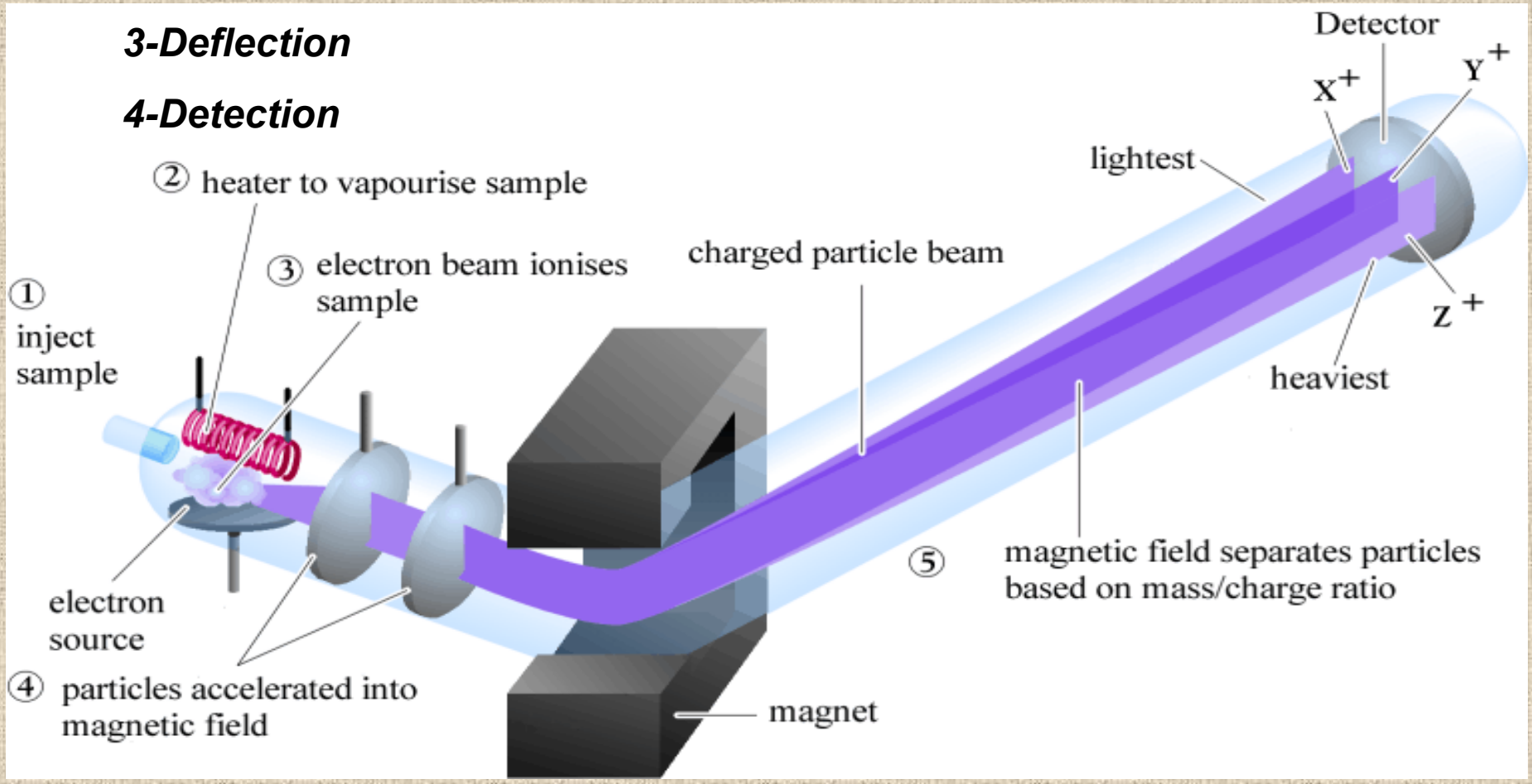
There are four stages in mass spectroscopy;

1-Ionisation

2-Acceleration

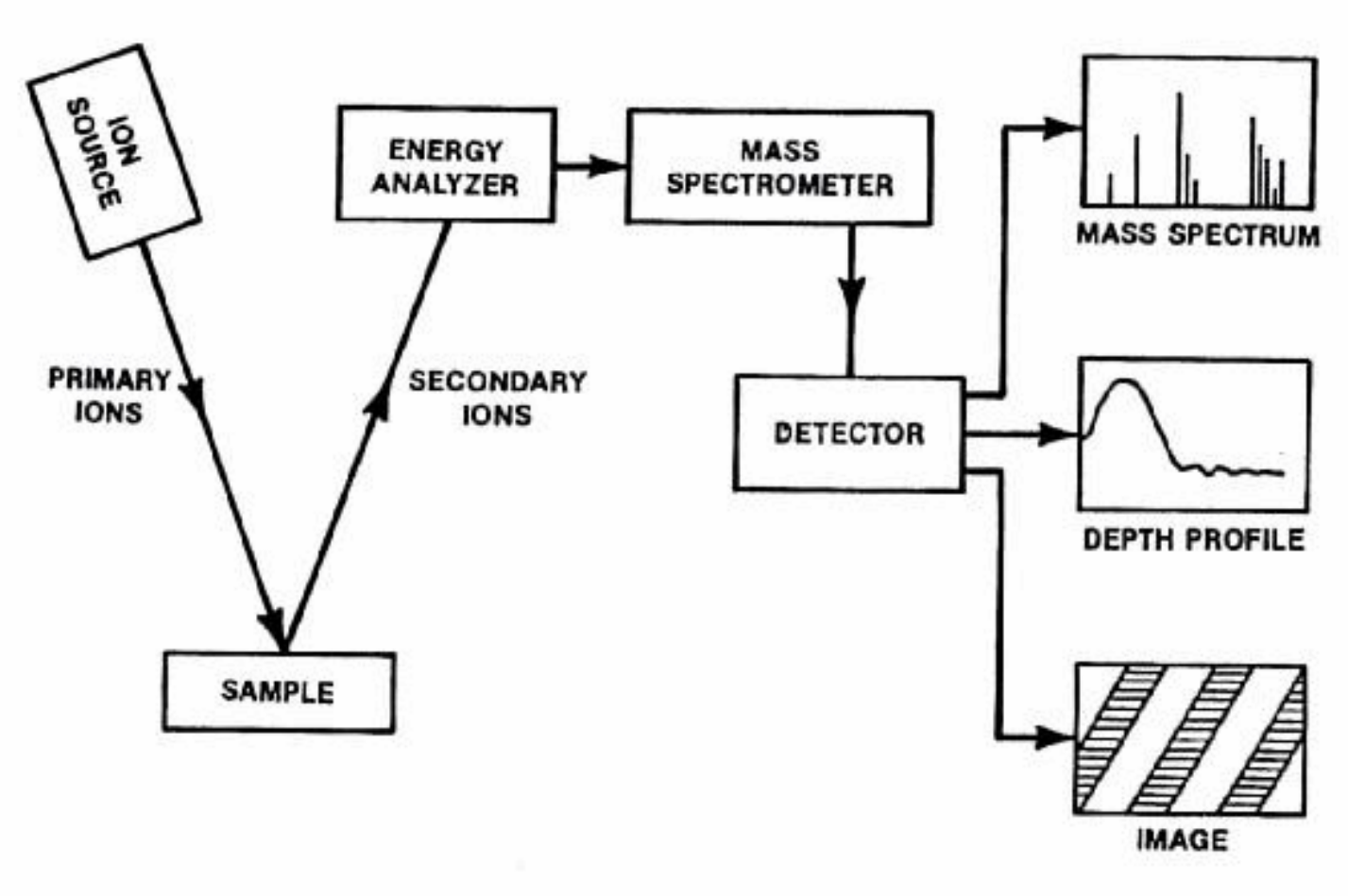
3-Deflection

4-Detection

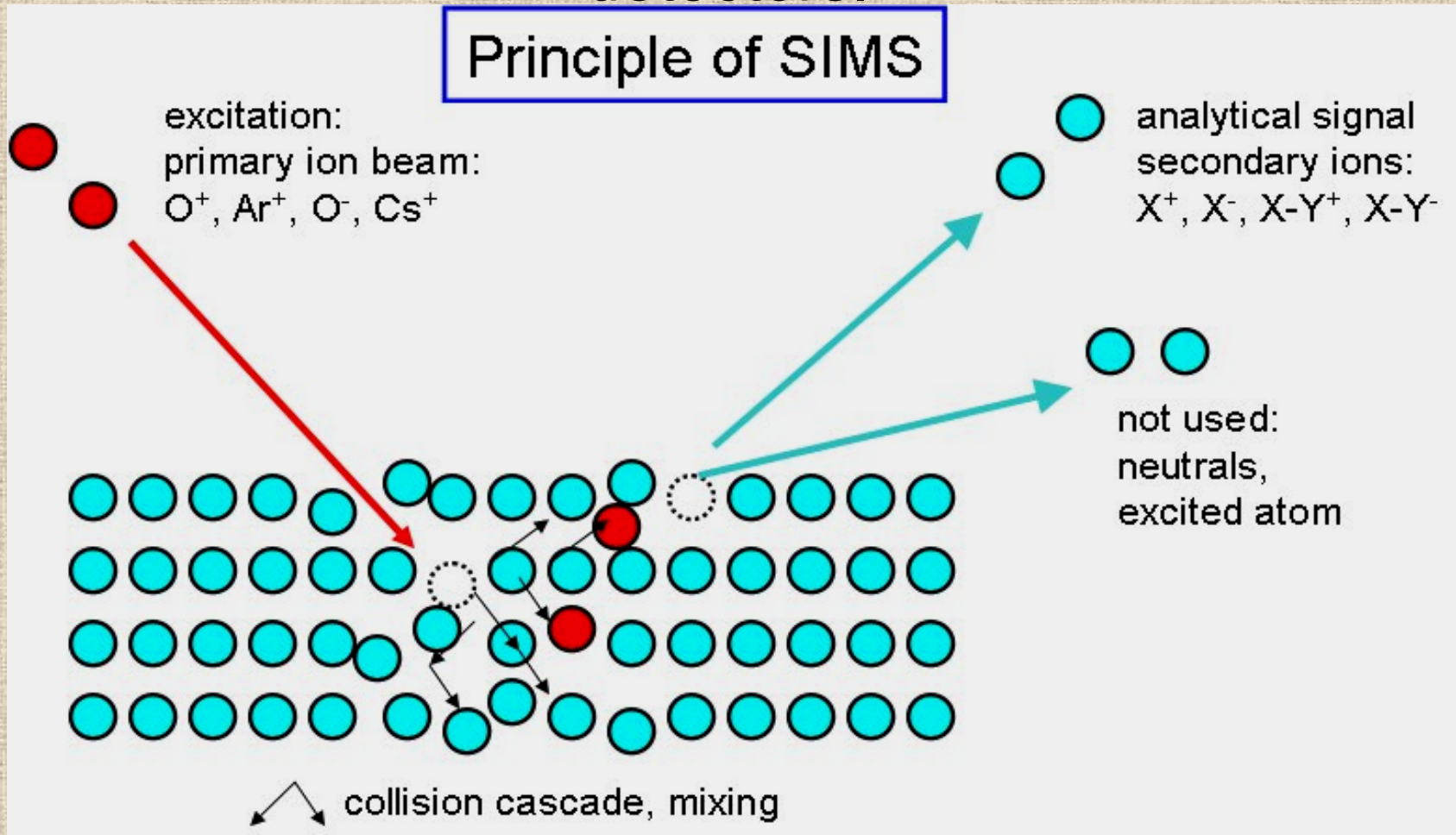


Secondary ion mass spectroscopy

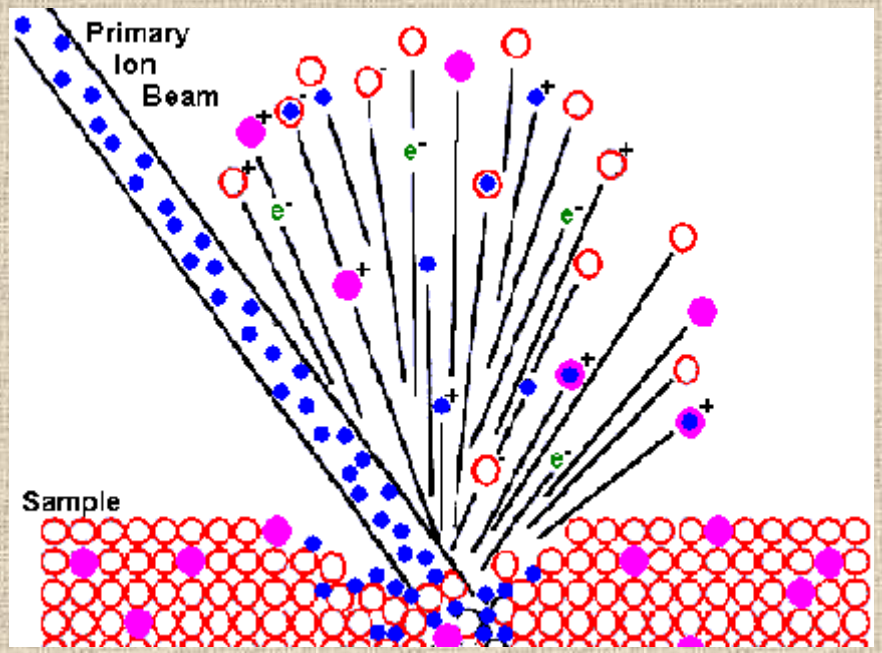
Basic Overview



By the interaction of the primary beam,most atoms and molecules removed from the sample acording to their masses and counted with suitable detectors.



Secondary ion generation



- The sample is prepared in an ultra high vacuum.
- A beam of primary ions or neutral particles impacts the surface with energies of 3-20 keV.
- A primary ion or particle causes a collision cascade amongst surface atoms and between 1 and 10 atoms are usually ejected. This process is termed sputtering. The sputter yield depends on the nature of the analyte.

Typically, a secondary ion mass spectrometer consists of:

- primary ion gun generating the primary ion beam
- primary ion column, accelerating and focusing the beam onto the sample (and in some devices an opportunity to separate the primary ion species by Wien filter or to pulse the beam)

- high vacuum sample chamber holding the sample and the secondary ion extraction lens
- mass analyser separating the ions according to their mass to charge ratio
- ion detection unit.

The Main Advantages and Disadvantages of MS and SIMS

Major Advantages of Mass Spectroscopy

- Provides molecular weights of peptides and proteins with high accuracy (0.1-0.01%)
- Highly sensitive
- Sample purity not important
- Can be coupled with on-line separation methods such as HPLC and capillary electrophoresis for the analysis of mixtures

Nu plasma MC-ICPMS.

http://serc.carleton.edu/images/research_education/geochemsheets/techniques/nuplasma1.jpg

Major Disadvantages of Mass Spectroscopy

- Noncovalent complexes are often disrupted
- Cannot distinguish stereoisomers
- Expensive instrumentation
- Few for proteins and peptides, as purity and sample requirements are not restrictive (fmol-pmol quantities can be used)
- Other biopolymers (nucleic acid, carbohydrates) are more difficult to analyze.

Major Advantages of Secondary Ion Mass Spectroscopy

- The possibility to detect all elements, beginning with H, and their isotopes
- The surface sensitivity
- Excellent depth resolution, good lateral resolution and
- Detection limits in the ppb range.

Major Disadvantages of Secondary Ion Mass Spectroscopy

- Sample consumption,
- Need of ultra high vacuum (samples have to be vacuum compatible, flat and, ideally, conductive)
- Some serious problems with regarding quantification.

Applications of MS and SIMS

- In general, the properties about atom and molecules can be learned with these methods.
- Mass spectrometry is used to determine the isotopic composition of elements within a sample.
- Pharmacokinetics is often studied using mass spectrometry.
- Characterization of proteins.

http://cmm.mrl.uiuc.edu/images/SIMS_640x480.jpg

- Mass spectrometers are sensitive detectors of isotopes based on their masses. They are used in carbon dating and other radioactive dating processes.
- Analyzing biological materials(SIMS)
- The investigation of possible links between glass failure and polishing residue in optical components used in powerful lasers(SIMS)

Thanks for listening..