Secondary Ion Mass Spectroscopy (SIMS)

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Several methods are available to characterize a surface chemically. STM allows in certain cases the identification of chemical elements via V-I spectroscopy. Data averaged across a bigger area and a better impression about the surface chemistry is obtained by AES. The depth of highest sensitivity can be adjusted via the primary electron energy within a few Å below the surface. If one wants a complete chemical depth profile, layer by layer can be sputtered away, while each sputtering process is followed by an AES measurement. When a mass-spectrometer is available one can also use material sputtered away to obtain information about the surface chemistry. This method (SIMS) allows to identify elements and how they are chemically bonded. A resolution in the order of a monolayer and a sensitivity of one ppm can be achieved. See Fig. 1 for a typical SIMS setup.

Sputtering is a series of two-body collisions. Depending on the ion energy three regimes can be distinguished:

1. For ion energies below $1\,\mathrm{keV}$ no recoil cascades will occur ("single knock-on regime").
2. For ion energies within the range of $1\,\mathrm{keV}$ to $1\,\mathrm{MeV}$ recoil atoms will produce further recoils ("linear cascade regime").
3. For ion energies above $1\,\mathrm{MeV}$ a certain volume around the impact of the ion is vaporized ("spike regime").

Typical sputtering ions for SIMS have an energy of $1\,\mathrm{keV}$ to $10\,\mathrm{keV}$. The sputtering occurs at an area in the order of $0,1\,\mathrm{mm}^2$. One has to take into account, that not all parts of the surface are sputtered evenly well. The sputtering yield varies from element to element. This leads to a convolution of the measured data with the sputtering probability. The spectrum is convoluted with the ionization probability, too. This depends on the chemical structure of the surface. Furthermore the argon ions used for sputtering can lead to ion implantation, destruction of the crystallographic order near the surface (see Fig. 2). Note, that the energy of the argon ions is sufficient to crack chemical bonds.

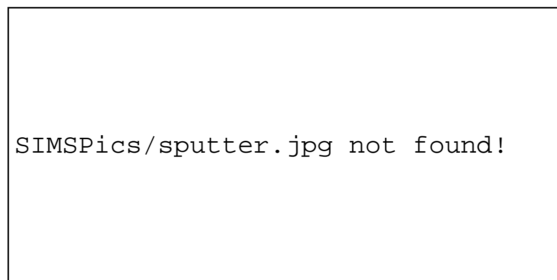

Figure 2: Schematic representation of the sputtering process, Fig. taken from [1].

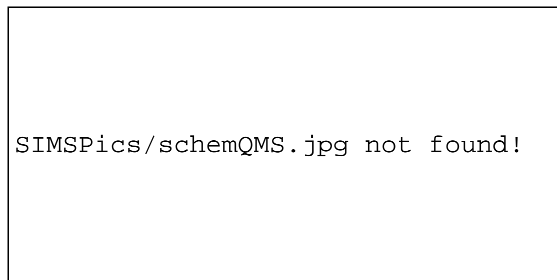

Figure 3: Schematic representation of a QMS, Fig. taken from [1].

The high sensitivity of SIMS if achieved through the use of a quadrupole mass spectrometer (QMS). It consists mainly of four parallel rods. They are electrically connected to two pairs. Between the pairs the sum of a AC and a DC voltage is applied. See Fig. 3 for a schematic representation.

The ions pass the QMS in the center of the rods. The

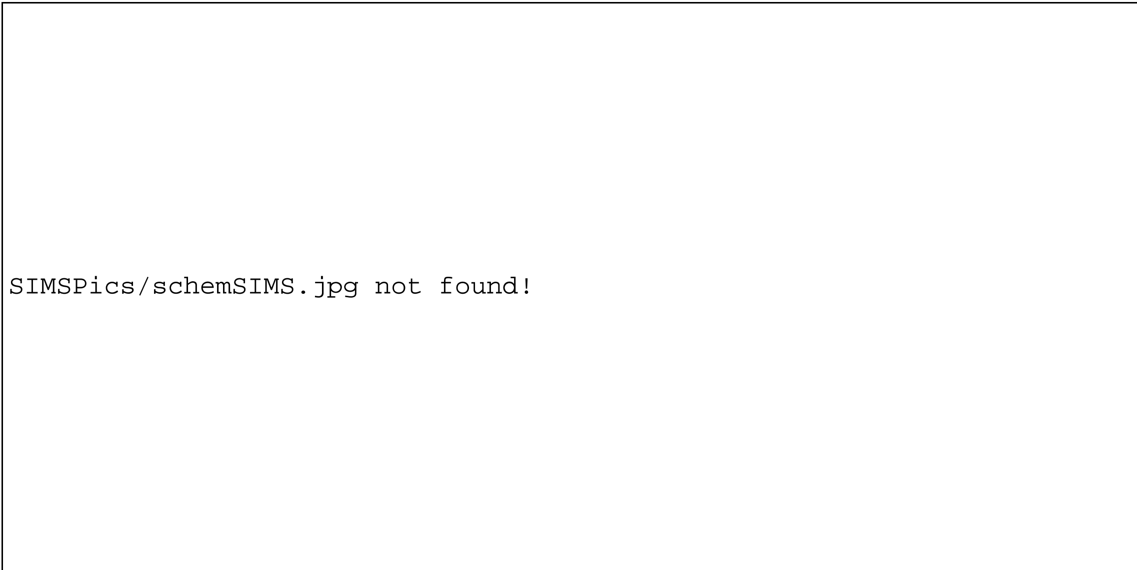

Figure 1: Typical SIMS Setup, Fig. taken from [1].

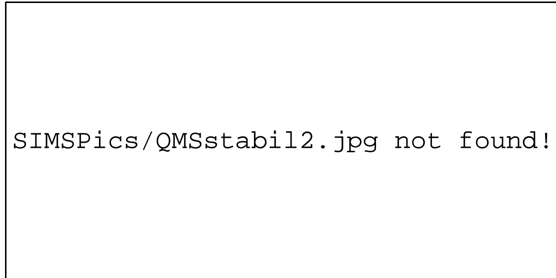

Figure 4: Stable and unstable solutions of the Mathieu Equations, Fig. taken from [2].

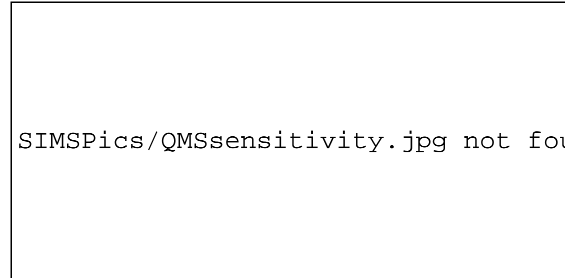

Figure 5: Typical transmission ratio of a EMS, Fig. taken from [1].

following dynamic equations can be obtained:

$$\begin{aligned}\ddot{x} + \frac{q}{mr^2}(U + V \cdot \cos\omega t)x &= 0 \\ \ddot{z} - \frac{q}{mr^2}(U + V \cdot \cos\omega t)z &= 0\end{aligned}$$

Substitution with $a = \frac{4qU}{mr^2\omega^2}$; $b = \frac{2qV}{mr^2\omega^2}$; $\tau = \frac{1}{2}\omega t$ leads to the Mathieu Equations. They have stable and unstable solutions. This behavior can be plotted depending on the parameters a and b (see Fig. 4). It is independent from the initial conditions. This “window” of stable solutions can be understood as follows: Ions with high masses can not follow the oscillatory electrical field and their trajectory will hit a rod of the QMS. Ions with low masses will oscillate with such high amplitudes, that they will also hit a rod.

Between the QMS and the ion detector an electrostatic mirror is placed. This reduces the background noise, because neutrals and photons will not contribute to the count rate. For quantitative measurements the QMS has to be calibrated (see Fig. 5).

Depending on the sputtering rate one distinguishes two modes of SIMS: Static SIMS with a current of 10^{-9} to 10^{-10} A/cm^2 corresponding to a sputtering rate of only 10^{-4} to 10^{-5}monolayers per second. The accompanying destruction is very minor, only the topmost layer is studied. Typical applications are the investigation of surface compostion, adsorption and surface

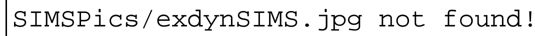

Figure 6: Nipi doped GaAs crystal with periods of 800 Å. p-doping was performed with carbon, n-doping was done with Si, Fig. taken from [1].

chemical reactions. The QMS must be very sensitive.

Dynamic SIMS works with a sputtering speed of several monolayers per second at ion currents from $10^{-4}$to 10^{-5} A/cm^2. Normally several mass spectra are recorded simultaneously. The sputtering rate limits the depth resolution, due to mixing of atoms from several layers within the detector. See Fig. 6 for an example of dynamic SIMS on a nipi doped GaAs crystal.

References

[1] H. Lüth, *Solid Surfaces, Interfaces and Thin Films*, 4th Edition, 2001, Springer, Berlin

[2] W. Demtröder, *Experimentalphysik 3,* 2th Edition, 2000, Springer, Berlin