Interaction of different $SrTiO_3$ surfaces with reactive gases

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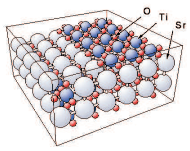
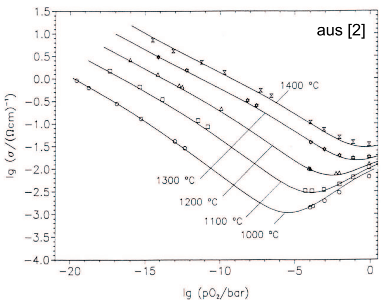
Introduction



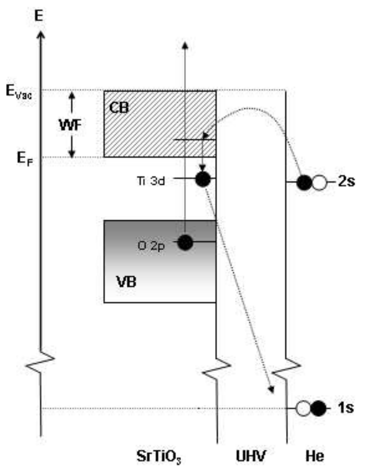
Donor doped Strontium Titanate is well known for its capability as resistive high temperature oxygen sensor. An interesting application of this sensor would be the analysis of automobile exhaust, as it would allow the optimisation of fuel injection and of catalytic oxidation of toxic exhaust, thus reducing fuel consumption and pollution of the environment. Before this application can be implemeted, preliminary studies aiming at the interaction of $SrTiO_3$ with reactive gases must demonstrate the stability of the material in this environment. Also, the influence of these gases on the interaction with oxygen must be clarified.



We use Metastable Impact Electron Spectroscopy and Ultraviolet Photoelectron Spectroscopy to analyse the valence band structure of $SrTiO_3$ and its adsorbates. X-ray Photoelectron Spectroscopy is used to check the stoichiometry of the samples. Our results for the interaction of $SrTiO_3$ with CO, CO_2, H_2O, CH_4 and other reactive gases being part of automobile exhaust are presented in this poster. We use $SrTiO_3$(100) as model substance und compare our results with experiments on polycristalline $SrTiO_3$ produced via a sol-gel route.

Experimental technique

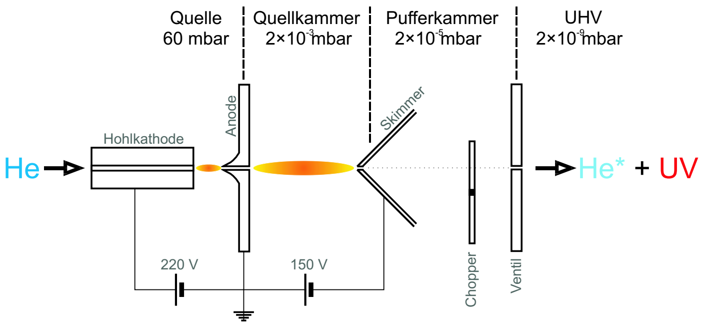
Metastable Impact Electron Spectroscopy (MIES) uses metastable He*($1s^1 2s^1$) to probe the surface of solids. The excitation potential of the He* amounts to 19.8 eV. Because the He* atoms interact with the surface in distances typically between 0.3 and 0.5 nm in front of it, MIES is extremely surface sensitive and displays the SDOS of the uppermost layer of the sample only. The interaction may proceed via different mechanisms.



During Auger Deexcitation (AD), an electron from the sample surface fills the 1s orbital of the impinging He*. Simultaneously the He 2s electron is emitted carrying the excess energy. The resulting spectra directly display the surface density of states (SDOS). To distinguish surface from bulk effects, AD-MIES and Ultraviolet Photoelectron Spectroscopy (UPS) can be compared directly.

For $SrTiO_3$, the He* interacts with the surface via the process shown on the left. The 2s electron of the impinging He* is resonantly transferred into the surface of the sample and localizes at near surface Ti 3d states. Subsequently, a Ti 3d electron fills the hole in He+ 1s in an interatomic Auger Neutralization (AN) process, followed by the emission of an O 2p surface electron carrying the excess energy. The energy of the resulting MIES peak is shifted by 1.2 eV toward higher binding energies compared to AD due to a diminished local ionization potential. A detailed discussion of this process is given in [1].

Our experimental setup is shown below. It produces He* for MIES as well as ultraviolet light for UPS, thus allowing to measure MIES and UPS simultaneously.



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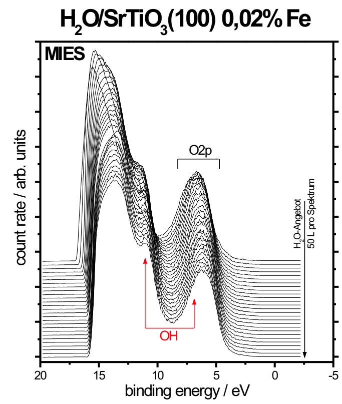
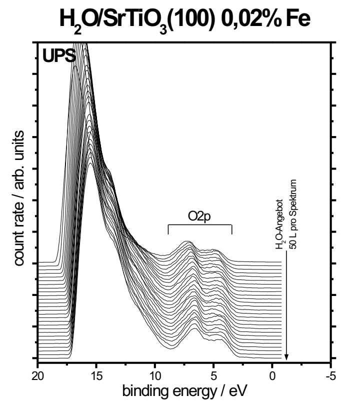
Atom- und Molekülphysik an Oberflächen

$SrTiO_3$ single crystals



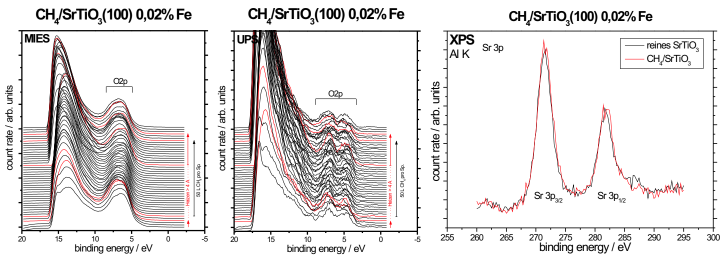


Experiments with $SrTiO_3$(100) single crystal surfaces under UHV conditions are currently in progress. Shown above is the reaction with water at room temprature. As can be seen, H_2O is partly dissociated and adsorbs as OH on the surface, creating the denoted structures in MIES. Molecular adsorbtion is not observed. The structure labelled O 2p is due to the modified AN process described before. UPS shows the valence band structure of $SrTiO_3$ and no further contributions. The OH decoration of defects and steps can be removed by mild heating of the $SrTiO_3$.

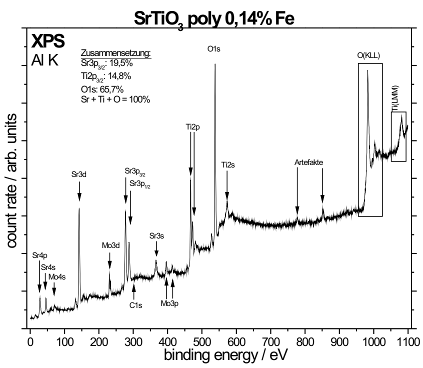
Shown below is an experiment where CH_4 was offered to the surface at about 500 °C. The MIES and UPS shows no interaction taking place. This result was confirmend by XPS.

So far, we couldn't find singnificant interaction between the $SrTiO_3$ surface and CH_4, CO and CO_2 in the temperature range between room temperature and 1000 °C. During some experiments with high pressure (up to 1000 mbar) at room temperature, an carbonate like structure seems to form. This contamination can be removed from the surface by mild heating.

Experiments in the near future will address the possible interactions at pressures up to 100 mbar and the reaction with NO, NO_2, H2S and So_2.



Polycristalline $SrTiO_3$

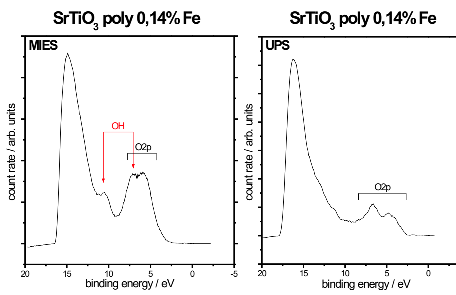


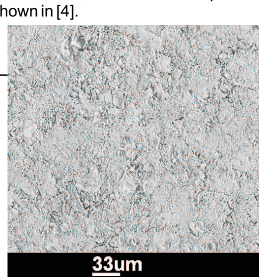
Polycristalline $SrTiO_3$ thin films were prepared by means of a modified Pecchini method (sol-gel technique).

The picture below shows a very rough surface, but covering the hole substrate and without macroscopic defects. The XPS measurement on the left was conducted on the same sample and shows the capability of the method to produce $SrTiO_3$ films with correct stoichiometry.

The MIES and UPS measurements in the lower left corner were taken after a longish heating procedure. Both methods show the correct structure as known from the single crystals, but an slight contamination with OH can still be detected with MIES.

Experiments in the future will address the reactions of such surfaces with reactive gases in the same manner as on the single crystals. Polycristalline or nanocrystalline $SrTiO_3$ films are a promising candidate for cheap and highly effective oxygen sensors, due to their improved dissoziaton capability and easy handling. First experiments are shown in [4].





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