

# Summary

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A broad spectrum of physical properties is exhibited by complex transition metal oxides with a perovskite crystal structure and this makes this group of materials very attractive for micro-electronic devices, specially when a combination of properties is wanted for an application. The extensive list of physical properties exhibited is partly due to the ability of the perovskite structure to accommodate almost every element of the periodic table.

In this thesis a relatively new type of transition metal oxide substrate surface is investigated, the (110) surface of the rare earth scandate  $\text{DyScO}_3$ . Besides the bare substrate surface, the growth kinetics together with the resulting film properties of  $\text{SrTiO}_3$  thin films deposited with Pulsed Laser Deposition (PLD) is investigated. To be able to fully investigate the deposition process a new and versatile PLD chamber was developed for use at the European Synchrotron Radiation Facility (ESRF). It allows for *in-situ* surface X-ray diffraction (SXRD) measurements during and directly after the deposition. With respect to other developed PLD-chambers for use at synchrotrons, the design described in this thesis allows for full crystallographic data acquisition over a wide angular range without any blind spots, thus yielding access to a large fraction of reciprocal space. The chamber can accommodate multiple targets, while the mounting of the laser on a common platform with the chamber minimises laser alignments. Experiments on two different beamlines at the ESRF (BM26 and ID15) show the new PLD-chamber functions well within its required specifications.

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Before a thin film of  $\text{SrTiO}_3$  can be deposited, however it is important to characterise the bare  $\text{DyScO}_3(110)$  surface. After the  $\text{DyScO}_3(110)$  crystal surfaces are cleaned and annealed yielding straight and equidistant step edges, the first impression given by Atomic Force Microscopy (AFM) is a single terminated surface with steps that are half a unit cell high. Growth experiments with  $\text{SrRuO}_3$  and SXRD experiment on the annealed substrates show that this is not the case and that the surface of annealed  $\text{DyScO}_3(110)$  has in fact a mixed termination. The complexity and surface disorder of the annealed  $\text{DyScO}_3(110)$  surface make it impossible to derive a model that fits all the SXRD data perfectly. Instead, a simple model is derived that agrees with most of the SXRD, AFM and growth data. It consists of a  $\text{ScO}_2$  single terminated surface with four partially occupied surface layers (i.e. one full unit cell of  $\text{DyScO}_3$ ) on top, with a displacement of the dysprosium atoms in the the first surface layer. The reason why this mixed termination of the annealed  $\text{DyScO}_3(110)$  surface is not seen with AFM is probably that the four partially occupied surface layers are present as surface features below the lateral resolution of the AFM.

With an improved sample preparation technique it is possible to obtain a  $\text{DyScO}_3(110)$  surface that is single,  $\text{ScO}_2$  terminated. After annealing the sample is subjected to a selective etching procedure using HF and NaOH. HF roughens the substrate first, making the subsequent NaOH etching step more effective and reliable. SXRD and Angle-Resolved Mass Spectroscopy of Recoiled Ions (AR-MSRI) data confirm the single  $\text{ScO}_2$  termination.

A single terminated  $\text{DyScO}_3(110)$  surface is polar. The surface structure is therefore investigated to explain how it is altered to avoid a polar discontinuity. Reflection High-Energy Electron Diffraction (RHEED) and SXRD data show no surface reconstruction for  $\text{DyScO}_3(110)$ , indicating the absence of systematic cation vacancies at the surface. Moreover, SXRD data indicate that cation displacements in relation to the bulk plane are unlikely to be present. Therefore, the polarity difference between bulk and vacuum is most likely overcome by introducing oxygen vacancies in the topmost Sc layer. However, the techniques used are not sensitive enough to confirm this.

The strain state of a  $\text{SrTiO}_3$  thin film is one of the interesting features of this system. As can be seen from measurements directly after deposition at  $700^\circ\text{C}$ , most of this strain is instantly present in the thin film. Assuming that the  $\text{SrTiO}_3$  thin film grows coherently on the substrate, almost all the

in-plane strain is already present at these elevated temperatures. For the out-of-plane direction a compression factor of about 0.96(9)% is measured, resulting in an out-of-plane lattice constant for the strained  $\text{SrTiO}_3$  thin film of 7.840(7)Å and a axial strain of -0.0023(9), about half the strain value compared to room temperature. Though most of the strain is present at elevated temperature the thin film is still expected to be in its paraelectric state, because the Curie temperature is below 450 °C.

When depositing  $\text{SrTiO}_3$  on  $\text{DyScO}_3(110)$ , the starting condition of the substrate can significantly influence the growth. When observing the growth oscillations of a deposition, in some cases the regular oscillatory behaviour is not observed right from the start. This initial stage was investigated in detail for the growth of  $\text{SrTiO}_3$  on annealed  $\text{DyScO}_3(110)$ . In this case the growth starts with the linear fill-up of the uncompleted surface layers of the substrate. This indicates a fast incorporation of the incoming adatoms into the thin film system, made possible by roughness of the uncompleted surface layers. After these layers of the substrate are almost filled up,  $\text{SrTiO}_3$  starts to grow in a layer-by-layer fashion in which only one  $\text{SrO}$  and one  $\text{TiO}_2$  layer grow simultaneously.