Report Proposal HC 4973: **Structural study of phase transitions in V_2O_3 under tensile and compressive strain**

Abstract

Vanadium sesquioxide (V_2O_3) undergoes a non-isostructural metal-insulator transition (MIT) at 160 K upon cooling from a corundum paramagnetic metallic (PM) phase to a monoclinic antiferromagnetic insulating phase (AFI), yielding a resistivity change of 7 orders of magnitude. Very recently, a room temperature (RT) paramagnetic metal-insulator (PM-PI) transition both in pure and Cr-doped V_2O_3 thin films induced by strain engineering has been reported by the proposers (P. Homm et al., APL Materials **9**, 021116 (2021)). Novel intermediate states between the PM and PI phases in both pure and Cr-doped V_2O_3 , inaccessible in bulk materials, can be stabilized by a fine tuning of the lattice parameter by engineered substrates. The detailed knowledge of atomic positions and corresponding evolution of lattice deformations across this iso-symmetric Mott phase transition are therefore extremely relevant for a deeper understanding of the interplay between lattice and electronic degrees of freedom in this Mott material.

The aim of this proposal is to study the structural properties as a function of temperature in V_2O_3 layers under both compressive and tensile strain induced by smart engineering of substrate templates. For this, we will analyze a series of V_2O_3 thin films grown epitaxially on $(Fe_yCr_{1-y})_2O_3$ (with y = 0.25, 0.5, 0.75 and 1) buffer layers. The proposed experiments will deepen the understanding of the relationship between structural and electronic properties in this strongly correlated material. By measuring samples with different amount of strain we will be able to study the structural changes across the transition from the PM, PI and intermediate states to the low temperature AFI phase. This proposal will complement the results obtained during the previous experiment done at BM25 SpLine "Structural and composition study of the room temperature metal-insulator transition in V_2O_3 thin film compounds" (Experiment 25-02-1000) where reciprocal space maps for pure V_2O_3 films grown on $(Fe_yCr_{1-y})_2O_3$ with y = 0.5, 0.75 and 1 were obtained at room temperature.

Experimental results

The samples studied in this beamtime were:
- P0034 (65 nm V_2O_3 on $(Fe_{0.75}Cr_{0.25})_2O_3/Cr_2O_3/Al_2O_3$)
- P0035 (65 nm V_2O_3 on $(Fe_{0.5}Cr_{0.5})_2O_3/Cr_2O_3/Al_2O_3$)
- P0033 (65 nm V_2O_3 on Al_2O_3)
- VO14 (62 nm V_2O_3 on Cr_2O_3/Al_2O_3)

High-angle diffraction and reciprocal space maps were performed in all samples as a function of temperature to study the structural evolution of the low temperature metal-insulator transition for different amount of strain. The chosen temperatures were: 300 K, 200 K, 180 K, 160 K, 140 K, 120 K, 100 K, 80 K, 60 K and 12 K.
In a previous beamtime we have observed, both V_2O_3 samples on Al_2O_3 and on Cr_2O_3/Al_2O_3 substrates, the formation of a structure different than the expected monoclinic one when cooling the high temperature corundum metallic phase. In those experiments the lowest

temperature studied was 80 K where this phase characterized by formation of three diffraction peaks in the ab-plane oriented at 120° from each other at temperatures around 160 K. During this new beamtime we were able to further explore the evolution of V_2O_3 crystalline structure down to 12 K. Reciprocal space maps were constructed by a series of theta-scans around different reflections: (0 0 L), (1 1 10), (0 2 6), (1 0 10), (1 0 8) and (1 1 9). We have selected these reflections in order to perform a comprehensive analysis of the reciprocal space and be able to determine the atomic displacements and changes associated with the observed intermediate structure. In Figure 1 we show reciprocal space maps constructed as L-scans around the (1 0 10) reflection in samples with different amount of strain induced by the concentration of Fe in the $(Fe_yCr_{1-y})_2O_3$ buffer layer.

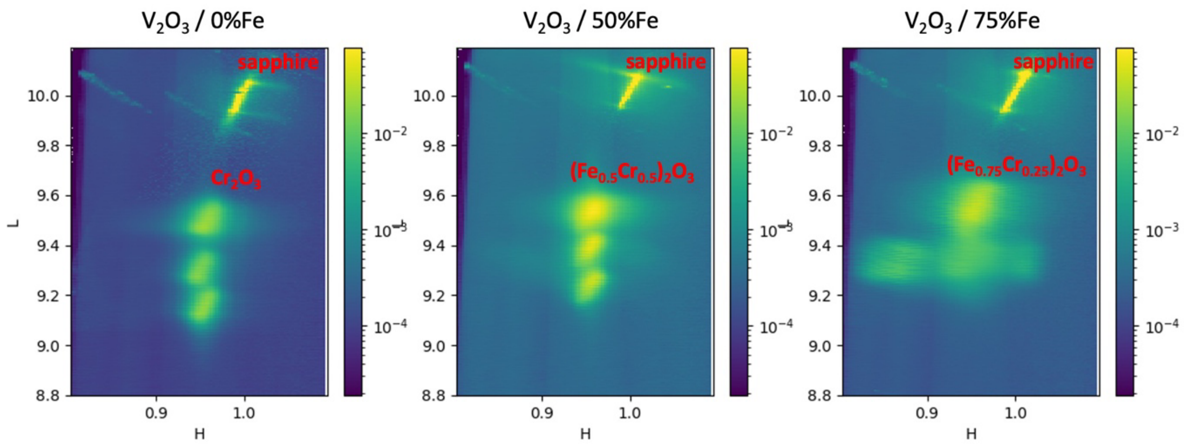

Figure 1. L-scans at 12 K around the (1 0 10) reflection on V_2O_3 subjected to strain induced by the Fe content (y) in the $(Fe_yCr_{1-y})_2O_3$ buffer layer.

Conclusions and future work

This experiment is related to previous experiments (25-02-956 and 25-02-1000) where we studied the temperature evolution of the structure of pure V_2O_3 films on Al_2O_3 and Cr_2O_3/ Al_2O_3 substrates and the room temperature structure of V_2O_3 films grown on $(Fe_yCr_{1-y})_2O_3$ buffer layers. These previous experiments have demonstrated that in V_2O_3 thin films the high temperature corundum (metallic) phase transforms in a low temperature monoclinic (insulating) phase via the formation of an intermediate phase. At the moment, we are dedicated to the thorough analysis of all the data collected during the beamtimes in order to unveil the structural characteristics of this intermediate state. All the RSMs collected on the samples with different amount of strain will allow us to determine the effect of strain in the resulting intermediate and low temperature phases. These results will be also analyzed in combination with studies of Far-infrared spectroscopy (FTIR) and Raman spectroscopy on the same samples in order to get a complete picture of the structural phase transition in (strained) thin films of V_2O_3. Preliminary results obtained during these beamtimes were presented as a poster in the 2022 IEEE- Semiconductor Interface Specialist Conference (7-10 December 2022, San Diego, USA): “Intermediate phase of V_2O_3 at low-temperature phase transition”, W.-F. Hsu, S. Mellaerts, M. Menghini, J. Rubio Zuazo, J. López Sánchez, J. W. Seo and J. P. Locquet.