ME1123 – Report

The analysis performed using Ifeffit has revealed two different kinds of crystalline network for our mesoporous V_2O_5 thin films, not ascribable to usual hydrous $V_2O_5 \cdot nH_2O$ or orthorhombic V_2O_5 phases. For our knowledge these particular crystalline structures have never been described before in literature.

EXAFS analysis was performed with the V_2O_5 orthorhombic phase lattice as reference. The results indicate a disordered 2D network where the nearest oxygen atoms are distributed on two doubly degenerate shells. The second neighbors shell is made by a single vanadium atom in the adjacent cell. The axial V=O bond is not revealed by EXAFS supporting the bi-dimensional character of this phase.

Results for this 2D phase are summarized and reported in Table 1 (from which is possible to underline a short range order in the equatorial plane for this network) and in Figure 1.

Paths	Feff0001 (V↔O)	Feff0003 (V↔O)	Feff0007 (V↔V)
R_{eff} (Å)	1.59	1.88	3.09
N legs	2	2	2
R (Å)	1.66	1.84	3.41
Degen	2	2	1
Amp	0.9	0.9	0.9
E_0 (eV)	-5.0	-5.0	-5.0
δR (Å)	0.07	-0.04	0.32
σ^2	0.002	0.005	0.005

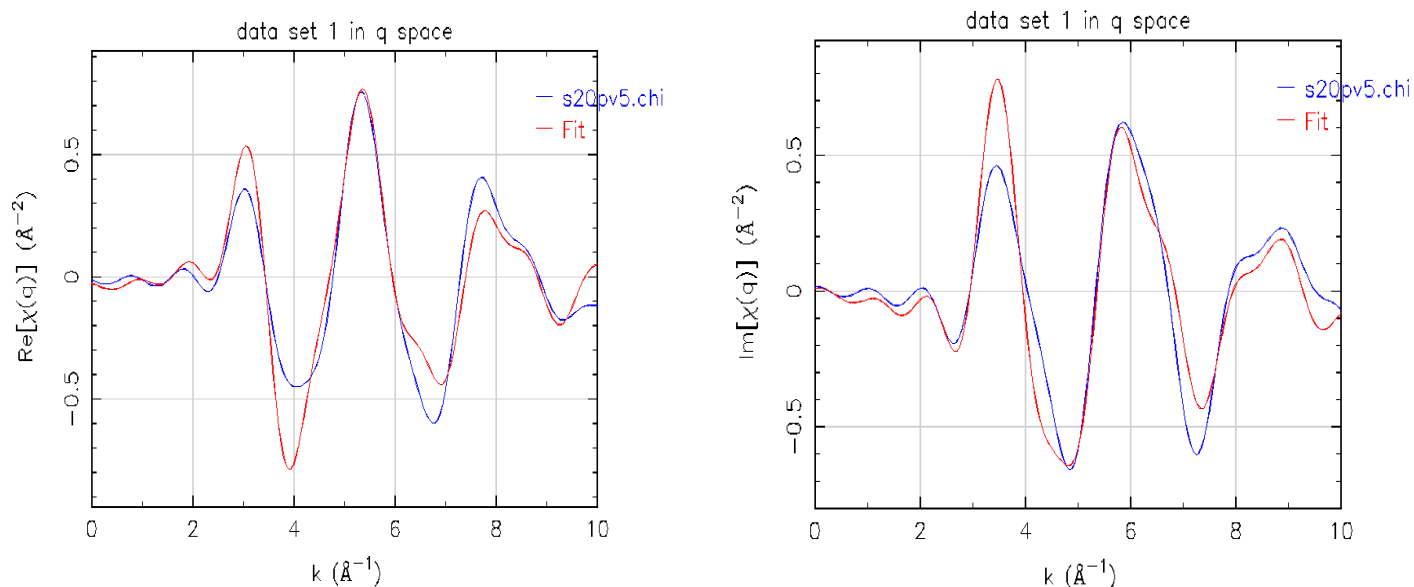**Table1.** Arthemis palettes from our best fit for this 2D phase.

Figure 1. Best fit in **q** space for the 2D VO_x network.

The other phase is characterized by a nearly 3D network, with both planar and axial order. The bond lengths are slightly different from those of orthorhombic V_2O_5 suggesting an intermediate phase between an hydrated $V_2O_5 \cdot nH_2O$ phase (2D) and the orthorhombic phase (3D).

In Table 2 and Figure 2 are reported and summarized results from our best fit for this phase.

Paths	Feff0001 (V<->O)	Feff0002 (V<->O)	Feff0003 (V<->O)	Feff0004 (V<->O)	Feff0005 (V<->O)	Feff0007 (V<->V)	Feff0013 (V<->V)
R eff (Å)	1,59	1,78	1,88	2,02	2,79	3,09	3,43
N legs	2	2	2	2	2	2	2
R (Å)	1,70	1,94	2,31	2,03	2,54	3,16	3,68
Degen	1	1	2	1	1	2	1
Amp	0,9	0,9	0,9	0,9	0,9	0,9	0,9
E0 (eV)	-5	-5	-5	-5	-5	-5	-5
dr (Å)	0,11	0,16	0,44	0,01	-0,25	0,07	0,25
σ2	0,006	0,006	0,006	0,006	0,006	0,006	0,003

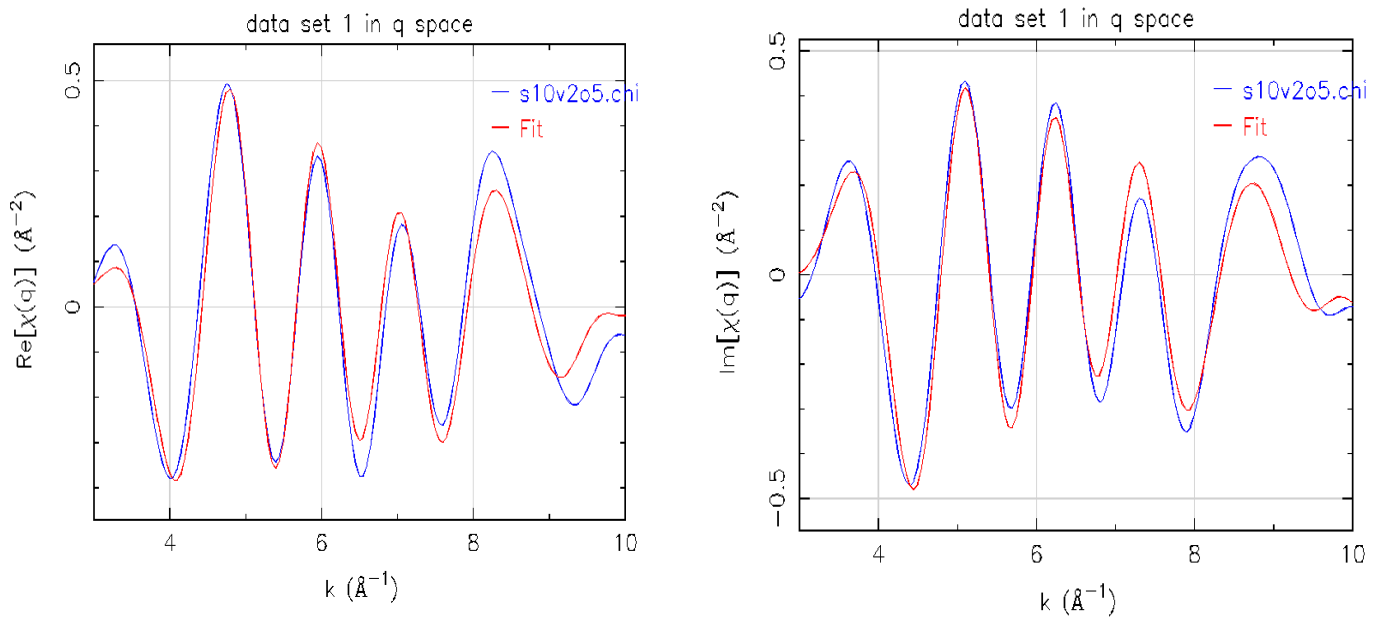**Table 2.** Arthemis palettes from our best fit for this phase.

Figure 2. Best fit in **q** space for the nearly 3D VO$_x$ network.

This work has been reported in the Poster Session of SAMIC 2005, held in Bressanone (Brixen), Italy, 4th-7th of September, 2005.

It will be presented in summary at the First International Conference on Nano-Structures Self-Assembling (NanoSEA), that will be held in Aix-en Provence, France, 2nd-6th of July, 2006.

A detailed report on this run of experiment will be presented at the European Conference on X-Ray Spectrometry (EXRS 2006), that will be hosted in Paris, France, 19th-23rd of June, 2006.