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Shifts: 18	Local contact(s): Valerio Sc	agnoli	ESRF GRenoble	Received at ESRF:
Names and affiliations of applicants (* indicates experimentalists):				
Dr. BLANCO Jesus Depart		partamento de Física. Universidad de Oviedo (Spain)		
Dr. LOVESEY Stephen ISIS Facility, Rutherford Appleton Laboratory (UK) and RIKEN SPring-8 Center, Harima Institute, (Japan) Dr. FERNANDEZ-RODRIGUEZ Javier Departamento de Física. Universidad de Oviedo (Spain)				
Dr. PAOLASINI Luigi E.S.R.F. Grenoble				
Dr. DE BERGEVIN François E.S.R.F. Grenoble				

Report:

Vanadium sesquioxide, V₂O₃, is an archetypal Mott-Hubbard metal-insulator [1] material that has been the object of intense study from the theoretical [3] and experimental [4] point of view in the last few decades. This compound has an interesting phase diagram, with an antiferromagnetic insulator phase (AFI) at low temperatures, and a paramagnetic metallic phase (PM) above the Néel temperature (T_N =150 K). The metal-insulator transition is accompanied by a strongly first-order structural phase transition in which the room-temperature corundum structure (R $\overline{3}$ c) is modified to monoclinic I2/a.

Recently, a new formulation of resonant x-ray Bragg diffraction by non-centrosymmetric materials was proposed by S.W. Lovesey et al. (unpublished) and applied to V_2O_3 . The purpose of this experiment has been to separate the contribution to scattering from the parity-odd E1-E2 mechanism, by measuring Bragg reflections where the parity-even E2-E2 contribution is predicted to be negligible.

Another motivation for this experiment on V_2O_3 is that, the parity-odd E1-E2 contributions to scattering, expressed in terms of anapoles, are of fundamental importance in current developments of the electronic structure of materials with magnetoelectric and ferroelectric modifications that are of potential technological interest.

The aim of this experiment has been to perform measurements on different space-group forbidden Bragg reflections at low temperature in the monoclinic phase. Together with energy profiles and azimuthal dependence, it was planned to measure the polarization dependence of a few "111-like" reflections by varying the incident linear polarization with phase plate. In this way, we can measure the Stokes parameters of the resonant reflection as a function of incident and scattered linear polarization angle, without cutting or moving the crystal. The great advantage is that the crystal is not moved in the observation, and data is collected on one micro domain of the crystal. With this method several forbidden reflections can be observed

within the same ESRF Experiment Description monoclinic domain.

For this experiment we have used a 2.8% Cr-doped $(V_{1-x}Cr_x)_2O_3$ (x=0.028) single crystal. The energy profiles of the space group forbidden reflections $(3,0,-2)_m$ and $(1,0,-2)_m$ were measured (Fig. 1), together with the azimuthal dependence of these reflections (Fig. 2) at a temperature T=100 K. The determined azimuthal dependence of $(3,0,-2)_m$ agrees with the result of a previous experiment done in year 2000, as it can be seen in Fig. 2a. The intensity in the reflection $(3,0,-2)_m$ comes mainly from the parity-even E2-E2 resonance, while the intensity in the $(1,0,-2)_m$ reflection comes from the parity-odd E1-E2 resonance.

It has not been possible to do measurements of the polarization dependence of the reflections using the phase plate due to the shortening in the available beam time produced by the cuts in the beam during the 19th November. It is planned to submit a proposal for a new experiment in 2007 for measuring the polarization dependence of space group forbidden reflections. This method can resolve resonances that are very close in energy, playing on their relative phase shifts [5]. It is also planned to complete the azimuthal angle scan measurements in the reflection $(1,0,-2)_m$ (only an interval of the azimuthal region in this reflection has been measured).

References

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[3] C. Castellani, C.R. Natoli, J. Ranninger, Phys. Rev. B 18(1978) 4945; 18 4967, 18 5001

[4] L. Paolasini, S. di Matteo, C. Vettier, F. de Bergevin et al. J. Electron Spectrosc. Relat. Phenom. **120**, 1 (2001).

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Fig. 1. Measured energy dependence of the $(3,0,-2)_m$ (1-a) and $(1,0,-2)_m$ (1-b) reflections at an azimuthal angle of $\psi = 0$ and at a temperature T = 100 K. Both polarization channels σ - σ and σ - π are shown.

Fig. 2. Azimuthal angle scans measured on the reflections $(3,0,-2)_m$ (1-a) showing data collected in the present experiment and data collected in a previous experiment done in 2001 (scaled to fit data from the present experiment), and $(1,0,-2)_m$ (1-b) at a temperature T=100 K. Both polarization channels σ - σ and σ - π are shown.