	Experiment title: Search of the experimental evidence of anapoles in V2O3	**Experiment number**: HE-3061
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Report:

Vanadium sesquioxide, V_2O_3, traditionally considered as a Mott-Hubbard metal-insulator system, has been the object of intense study [1-8]. This compound has an interesting phase diagram, with an antiferromagnetic insulating phase (AFI) at low temperatures, and a paramagnetic metallic one (PM) above the Neel temperature ($T_N \sim 150$ K). The metal-insulator transition is accompanied by a first-order structural phase transition in which the room-temperature corundum structure is modified to monoclinic I2/a. In 1978 Castellani, Natoli and Ranniger [1] proposed a theoretical model to explain the magnetic structure in the AFI phase from the ordering pattern of the occupation of the t_{2g} (degenerate) orbitals. This model was considered valid until 1999, when resonant x-ray diffraction [5], and magnetic dichroism [8] demonstrated that the spin of the Vanadium atoms was $S_V = 1$, whereas the model of Castellani predicted $S_V = 1/2$.

In vanadium sesquioxide V ions are located in crystal positions that are not a center of inversion symmetry, hybridization will occur between valence orbitals with different parity of that ion as a result of angular anisotropy in the cation's electron distribution from covalency and odd-order contributions in the electrostatic potential. This enables the possibility of observing electronic transitions to the hybridized states via the mixed dipole-quadrupole (E1-E2) channel in resonant x-ray scattering [9-10], which is sensitive to the ordering of parity-odd multipolar moments. For example, the ordering of magneto-electric anapolar moments might be observed. An orbital anapole moment characterizes a system that does not transform into itself under space inversion [9]. In the same way as parity-even contributions to resonant scattering can give information on different parity-even multipolar moments: dipoles, quadrupoles, hexadecapoles, etc., parity-breaking E1-E2 contributions to scattering can be expressed in terms of polar and magneto-electric tensors that contain the anapole operator. The study of these contributions to resonant x-ray diffraction is of fundamental importance in current developments of the electronic structure of materials with complex electronic properties, such as magnetoelectricity, piezoelectricity and ferroelectricity that are of potential technological interest. Anapolar moments in magnetic ions at noncentrosymmetric sites can play an important role in multiferroic properties.

In the AFI phase of V_2O_3 the magnetic structure is such that the I-centering cell translation is time inverting. Because of the magnetic moments being colinear in the a_m-c_m plane, normal magnetic peaks are observed only at reflections $(hkl)_m$ with even h even and odd (k + l). Yet, peaks have been measured at odd h, even (h + l), at the resonant prepeak of the Vanadium K-edge.

The aim of this experiment has been to study the influence of the applied magnetic field in the magnetic and crystalline structure of the AFI phase of V_2O_3. It has been planned to study the effect of the magnetic field H in the configurations with H parallel and perpendicular to the b_m monoclinic axis. A single crystal of 2.8% Cr-doped $(V_{1-x}Cr_x)_2O_3$ (x = 0.028) was mounted on the six-circle diffractometer with horizontal scattering geometry (incident polarization is π, parallel to the scattering plane). The sample was cooled in a displex cryostat down to 100 K, and a single monoclinic domain was obtained in the beam illuminated area. The V_2O_3 crystal was placed with its normal surface direction $<001>_H$ in the scattering plane.

Initially, the monoclinic b_m axis was maintained perpendicular with respect to the applied magnetic field, giving access to the set of $(h,k,-h)_m$ reflections, which include the Templeton reflections $(1,0,-1)_m$ and $(3,0,-3)_m$. It was planned to move the position of the monoclinic b_m axis by using the azimuthal stick to rotate the sample about the $<001>_H$ axis, and to study the effect of applying the external magnetic field parallel to the b_m axis. This would have given access to a different set of reflections including $(3,0,-2)_m$ and $(1,0,-2)_m$, which were measured in previous experiments without applied magnetic field. However, there was a malfunctioning of the motor of the azimuthal stick, which did not allow rotating the sample.

Energy profiles were measured at different reflections for different values of the magnetic field in the Hbm configuration for the reflections $(2,1,-2)_m$, (resonant magnetic scattering), $(3,1,-3)_m$, (produced by time-odd magnetoelectric tensors [9]) and $(3,0,-3)_m$ (Templeton scattering). The variation of the energy profiles with the magnetic field is shown below. While a change in the shape of the energy profiles when introducing the magnetic field is observed, no new features appear which would be a signature a change in the magnetic or crystallographic structures.

Fig. 1. Measured energy profiles at the space-group forbidden reflections $(2,1,-2)_m$ (a), $(3,1,-3)_m$ (b), and $(3,0,-3)_m$ (c) at different values of the applied external magnetic field H. The measurements have been done in the π-π' polarization channel. In these measurements the b_m monoclinic axis is contained in the plane of scattering.
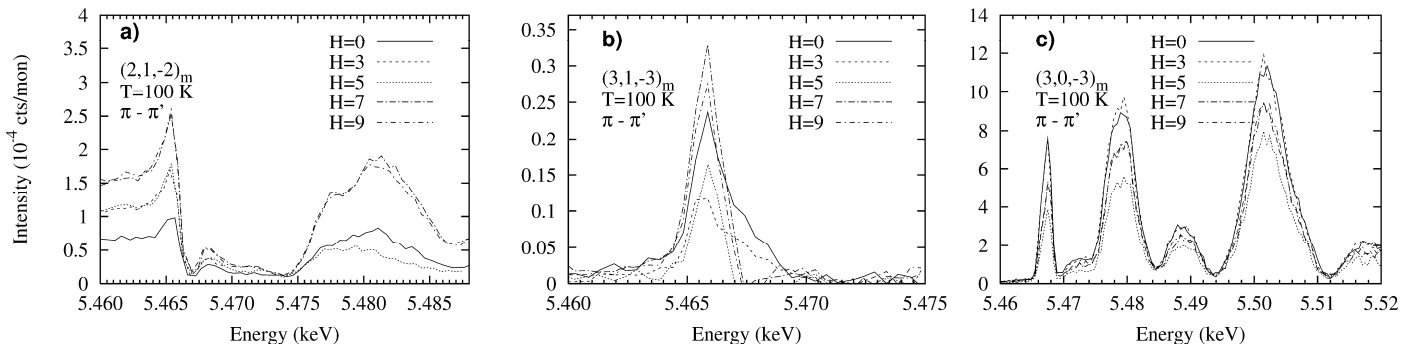
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