

**MS38 O1**

**Magnetic ordering in charge-ordered manganites: ionic vs Zener polarons pictures** Juan Rodríguez-Carvajal, *Institut Laue-Langevin, BP156, 38042 Grenoble Cedex 9, France.* E-mail: [jrc@ill.fr](mailto:jrc@ill.fr)

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In the  $R_{1-x}D_xMnO_3$  ( $R^{3+}$ ,  $D^{2+}$ ,  $x \approx 1/2$ ) manganites, belonging to the  $ABO_3$  perovskite family, the structural phase transition at  $T_{CO}$  is commonly interpreted (ionic picture) as a concomitant charge and orbital ordering (CO/OO) process driven by a co-operative Jahn-Teller effect and Coulomb repulsion forces. The low temperature phase is supposed to contain well separated  $Mn^{3+}$  and  $Mn^{4+}$  ionic species ordered in a well defined pattern [1, 2]. It is expected, from that model, that  $Mn^{3+}O_6$  octahedra should be strongly distorted and with average Mn-O distance around 2.02 Å, whereas  $Mn^{4+}O_6$  octahedra, having an average Mn-O distance of 1.90 Å, should be nearly undistorted. The so called CO transition may also be interpreted in terms of the formation of Zener polarons (ZP) that order spatially at  $T_{CO}$  [3]. This last picture combines the spatial ordering of the charge density with a partial delocalisation of electrons between few Mn-ions coupling them ferromagnetically. This last interpretation comes from the combination of a structural model obtained from single crystal neutron diffraction demonstrating that the expected distortions from the ionic picture do not occur [3] and the magnetic susceptibility of manganites in which  $T_{CO}$  is higher than the magnetic ordering temperature. In such compounds there are two paramagnetic regions separated by  $T_{CO}$ . The consequences of the ZP picture concerning magnetic ordering will be discussed. The talk will review what is known about the magnetic ordering in manganites, mostly around compositions close to half-doped; the problems related to the degeneracy of solutions in neutron powder diffraction giving rise to nearly the same diffraction pattern for physically different magnetic structures, and new results concerning the magnetic ordering in manganites without chemical disorder in the A-site.

[1] Goodenough, J. B., *Phys. Rev.* 1955, 100, 564.

[2] Radaelli P., Cox D.E., Marezio M., Cheong S-W., *Phys. Rev. B* 1997, 55, 3015.

[3] Daoud-Aladine A., Rodríguez-Carvajal J., Pinsard-Gaudart L., Fernández-Díaz M.T., Revcolevschi A., *Phys. Rev. Lett* 2002, 89, 097205

**MS38 O2**

**Probing Novel Order Parameters in Multiferroics with X-ray Resonant Scattering** D.F. McMorrow<sup>a</sup>, T. Beale<sup>d</sup>, S. Bland<sup>d</sup>, A.T. Boothroyd<sup>e</sup>, R. Ewings<sup>e</sup>, T.Forrest<sup>a</sup>, P.D. Hatton<sup>d</sup>, Y. Joly<sup>f</sup>, D. Mannix<sup>b</sup>, R., D. Prabhakaran<sup>e</sup>, H. Walker<sup>a</sup>, S.B. Wilkins<sup>c</sup>, <sup>a</sup>*Department of Physics, University College London, UK*, <sup>b</sup>*XMaS CRG Beam line, ESRF, France*, <sup>c</sup>*Brookhaven National Laboratory, USA*, <sup>d</sup>*Department of Physics, University of Durham, UK*, <sup>e</sup>*Clarendon Laboratory, University of Oxford, UK*, <sup>f</sup>*CNRS-Grenoble, Grenoble, France.*

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X-ray scattering techniques have been used to study the multiferroic compound  $TbMnO_3$ . A comprehensive set of experimental data will be presented, including non-resonant x-ray magnetic scattering and resonant scattering at the Mn (K and L) and Tb (L and M) absorption edges. From these measurements a complete description is obtained of the relevant order parameters in the different ordered phases of  $TbMnO_3$ . A critical discussion will be given of how these data relate to the known magnetic and structural properties of  $TbMnO_3$ , and to theories of the origin of multiferroicity in this compound.

**MS38 O3**

**Charge Ordering and Isosymmetrical Phase Transitions in Mixed Valence Vanadates  $MV_4O_8$  ( $M=Y, Yb$ )** Karen Friese<sup>a</sup>, Yasushi Kanke<sup>b</sup>, Andy N. Fitch<sup>c</sup>, Andrzej Grzechnik<sup>a</sup>, <sup>a</sup>*Department of Condensed Matter Physics, University of the Basque Country, Bilbao, Spain*; <sup>b</sup>*Advanced Materials Laboratory, National Institute of Material Science, Tsukuba, Japan*; <sup>c</sup>*European Synchrotron Radiation Facility, Grenoble, France.* E-mail: [karen.friese@ehu.es](mailto:karen.friese@ehu.es)

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The  $\alpha$ - and  $\beta$ -phases of  $YV_4O_8$  and  $YbV_4O_8$  (space group  $P12_1/n1$  for the  $\alpha$ - and  $A2_1/d11$  for the  $\beta$ -phases) are composed of essentially identical  $V_4O_8$  octahedral frameworks and differ only in the arrangement of the trivalent cations [1,2]. As a consequence, one-dimensional disorder and a co-existence of the two polytypic modifications is frequently observed [3,4]. Magnetic susceptibility measurements show anomalies at approximately 190 K for  $\beta$ - $YV_4O_8$  and 183 K for  $\beta$ - $YbV_4O_8$ , which can be attributed to a paramagnetic-paramagnetic transition. At about 80 K, a further magnetic anomaly is observed for both compounds. For  $\alpha$ - $YV_4O_8$ , on the other hand, magnetic anomalies are observed at approximately 78 and 50 K (measurements for  $\alpha$ - $YbV_4O_8$  have not been performed yet).

To characterize the structural response to these magnetic transitions, powder diffraction diagrams of the four phases have been measured in the temperature range from 290 K to 10 K at the European Synchrotron Radiation Facility, Grenoble, France (the beamline ID31). Our studies show no indication of a change in symmetry for all four phases (space group  $P12_1/n1$  for the  $\alpha$ - and  $A2_1/d11$  for the  $\beta$ -phases) in the whole temperature range, yet significant discontinuities in the lattice parameters indicate that some of the magnetic anomalies are accompanied by isosymmetrical phase transitions.

In addition, single crystal diffraction experiments have been carried out on  $\beta$ - $YbV_4O_8$  at the Institute for Synchrotron Radiation (Karlsruhe, Germany). The results confirm the existence of an isosymmetrical phase transition at approximately 180 K, which can be attributed to charge ordering. In the high temperature phase, the four symmetrically independent V-sites are partially occupied by tri- and tetravalent vanadium ions. At the phase transition, the tetravalent vanadium concentrates on one octahedron (V21) while the three trivalent vanadium ions fully occupy the remaining octahedra. This charge ordering is accompanied by discontinuous changes in the V-V, Yb-Yb and Yb-V interatomic distances.