[2] T. Kimura, et al. Phys. Rev. B68, 060403(R)(2003).
[3] M. Mostovoy, Phys. Rev. Lett. 96, 067601 (2006).
[4] D. Senff et al. Phys. Rev. Lett. 98, 137206 (2007)
[5] O. Prokhnenko et al. Phys. Rev. Lett. 98, 057206 (2007)
[6] O. Prokhnenko et al. Phys. Rev. Lett. 99, 177206 (2007)

Keywords: multiferroics, electomagnons, neutron scattering

MS.74.4

Acta Cryst. (2008). A**64**, C127

Crystal and magnetic structures of frustrated antiferromagnet $CuCrO_2$

Françoise H. Damay[1], Gilles Andre[1], Maria Poienar[2], Christine Martin[2], Antoine Maignan[2]
[1]Laboratoire Leon Brillouin, CEA-CNRS UMR 12, Bat 563, CEA Saclay, GIF SUR YVETTE Cedex, Essonne, 91191, France, [2]Laboratoire CRISMAT, CNRS UMR 6508, ENSICAEN, 6 bvd Marechal Juin, 14050 CAEN Cedex, France, E-mail：francoise.damay@cea.fr

The crystal and magnetic structures of the frustrated antiferromagnet delafossite $CuCrO_2$ have been investigated by means of neutron powder diffraction between 1.5K and 300K. $CuCrO_2$ exhibits at 300K a highly anisotropic rhombohedral *R*-3*m* structure ($a = b =$ 2.976(1) Å and c = 17.109(1) Å), in which compact CrO_6 layers are separated by linearly coordinated Cu+ ions. Within the instrumental resolution, no crystal structure transition is observed down to 1.5K. Below T_N = 27K, broad magnetic peaks appear, which can be indexed with an incommensurate propagation vector (q, q, 0), q ≈ 0.329. Using symmetry analysis [1], we found several possible models for the magnetic structure, some of them compatible with magnetoelectricity. It is noteworthy that, chromium species being distributed on a triangular lattice, the total spin on each triangle is roughly $\Sigma_i S_i = 0$, as expected for a frustrated antiferromagnet. Second order magnetic exchange between CrO_6 layers is probably responsible for the 3D ordering. The shape of the magnetic peaks can be well described by a model of magnetic platelets 200Å thick randomly stacked along *c* [2], which suggests that long-range order is finite in the *c* direction but well established in the *a*-*b* planes, in agreement with previous results [3]. Effects of various Cr-site substitutions on the magnetic ordering will also be presented.
[1] J. Rodriguez-Carvajal, BASIREPS
[2] J. Rodriguez-Carvajal, Physica B 192, 95 (1993)
[3] H. Kadowaki et al. J. Phys. : Condens. Matter 2, 4485 (1990)

Keywords: neutron powder diffraction, delafossite, magnetic structures

MS.74.5

Acta Cryst. (2008). A**64**, C127

Frustration of magnetic and ferroelectric long-range order in $Bi_2Mn_{4/3}Ni_{2/3}O_6$

John B. Claridge[1], Helen Hughes[1], Craig A. Bridges[1], Mathieu Allix[1], Mathew J. Rosseinsky[1], Dominique Grebille[2], Oliver Perez[2]
[1]University of Liverpool, Chemistry, Robert Robinson Laboratory, Liverpool, Merseyside, L69 7ZD, UK, [2]Laboratoire CRISMAT-ENSICAEN, UMR6508, 6 Bd du Marechal Juin, 14050 Caen Cedex, France, E-mail：claridge@liv.ac.uk

Attempts to design a multifunctional material that can be made under ambient conditions, yielded $Bi_2Mn_{4/3}Ni_{2/3}O_6$. The material adopts a perovskite related structure with Bi on the A-site and a random of 67% Mn and 33% Ni on the B-site. X-ray and neutron powder diffraction data appear to give an orthorhombic cell of $2^{1/2}a_p$, $2x2^{1/2}a_p$ and $4a_p$ ($a_p \sim 3.88$Å) and the polar $Pn2_1m$ space group. More detailed analysis of the room temperature phase showed that it is incommensurate and a more detailed description of the structure and properties is presented. Synchrotron x-ray diffraction and constant wavelength neutron diffraction on powder samples were analyzed using the superspace group *Ibmm*(0-β0,α00)gm.ss (a = 5.5729(1) Å, b = 7.7686(2)Å, c = 5.5091(2)Å, α = 0.4930(3), β = 0.4210(7)). This (3+2)D description is more consistent with the observed physical properties and the apparent low polarization, and shows that some Mn/Ni order is present. Impedance spectroscopy shows an anomaly in the dielectric constant between 150 and 240ºC. Which temperature dependent neutron powder diffraction data confirmed is associated with a structural transition to a $GdFeO_3$ type structure, though weak modulation peaks are observed at high temperature neutron diffraction consistent with either short range order or cation order. Magnetic measurements show spin-glass like behavior below 35K. Variable temperature neutron diffraction confirms the absence of long-range magnetic order, though there is an anomaly in the temperature dependence of the sub-cell parameters at the at the spin glass transition temperature.

Keywords: incommensurate structures, magnetic oxides, ferroelectric oxides

MS.75.1

Acta Cryst. (2008). A**64**, C127−128

Electron localization phenomena in complex carbides of rare earth and transition metals

Wolfgang Scherer[1], Volker Eyert[1], Georg Eickerling[1], Benjamin Rohrmoser[1], Rene Kaecke[1], Christoph Hauf[1], Rainer Poettgen[2], Christian Vogt[2], Rolf-Dieter Hoffmann[2], Ute Ch. Rodewald[2]
[1]University of Augsburg, Institute of Physics, Chair of Chemical Physics and Materials Science, Universitätsstr. 1, Augsburg, Bavaria, 86159, Germany, [2]Institut fuer Anorganische und Analytische Chemie, Westfaelische Wilhelms-Universitaet Muenster, Corrensstr.30, D-48149 Muenster, Germany, E-mail：wolfgang.scherer@physik.uni-augsburg.de

The nature of chemical bonding in the complex carbides $Sc_3[TM(C_2)_2]$ (TM = Mn, Fe, Co, Ni) has been explored by combined experimental and theoretical charge density studies.[1] The structures of these organometallic carbides contain one-dimensional infinite TC_4 ribbons embedded in a scandium matrix. The bonding in these carbides were studied experimentally by multipolar refinements based on high resolution X-ray data and compared to scalar-relativistic electronic structure calculations using the augmented spherical wave (ASW) method. Besides substantial covalent T-C bonding within the TC_4 ribbons one observes also discrete Sc-C bonds of noticeable covalent character. Furthermore, our study highlights that even tiny differences in the electronic band structure of solids might be faithfully recovered in the properties of the Laplacian of the experimental electron density. In our case, the lifting of the Fermi level in the Co(d^9) carbide 1 relative its isotypic Fe(d^8) species 2 is reflected in the charge density picture by a significant change in the polarization pattern displayed by valence shell charge concentrations of the transition metal centers in the TC_4 units (T = Fe, Co). Hence, precise high-resolution X-ray diffraction data provide a reliable tool to discriminate and analyze the local electronic structures of isotypic solids even in the presence of a severe coloring problem (Z(Fe)/Z(Co) = 26/27). Funding from the DFG priority program (SPP 1188) is greatfully acknowledged.
References: