

not yet reliable. We will demonstrate the protein crystallography by June with the improved machine and reduced background.

Keywords: synchrotrons, protein crystallography, EXAFS

MS.90.5

Acta Cryst. (2008). A64, C152

Integrating laser and linac technology for next generation X-ray sources

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We will discuss a superconducting linac-based compact inverse Compton scattering source of hard x-rays appropriate for a university or industry laboratory. The process of inverse Compton scattering, in which an electron of 20-50 MeV backscatters an optical photon into the hard x-ray spectral range, offers the opportunity to produce high-brilliance hard x-ray beams with a laboratory-scale facility. Using a 2-meter superconducting linac and a 1-kW laser system, the time-average brilliance of such beams will be similar to 2nd generation synchrotron facilities. Two important characteristics will make our concept unique in comparison to the best synchrotrons or other compact sources. First, beam size can be below 10 microns, and second, the pulse length can be as short as 100 femto-seconds opening up applications difficult or impossible with even 3rd generation sources. This talk will discuss the conceptual design of such a source and the scientific program it could support, including imaging and crystallography in both static and time-dependent modes.

Keywords: high-power lasers, Compton scattering, synchrotron radiation sources

MS.91.1

Acta Cryst. (2008). A64, C152

Liquid state of spins and charges in geometrically frustrated spinel oxides

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Among a wide variety of structural categories of transition metal oxides, the spinel, generally expressed by the chemical formula AB_2O_4 , is unique in that an extremely strong geometrical frustration on both "spin" and "charge" channels is anticipated from its pyrochlore B-sublattice, a corner shared network of B-tetrahedra. We have been exploring novel liquid states of spins and charges produced by frustration using spinel structure as a play ground. In this talk, we present recent highlights of such exploration. $Na_4Ir_3O_8$ with $S=1/2$ Ir^{4+} was discovered. This compound crystallizes in "hyper-Kagome" structure, which can be viewed as a cation-ordered (Ir and Na) spinel structure. We show that the ground state of this system is very likely a three dimensional $S=1/2$ spin liquid as a consequence of geometrical frustration [1]. LiV_2O_4 spinel is a "charge" frustrated system because of the mixed-valent configuration with 1:1 ratio of V^{3+} and V^{4+} , where we found a charge analogue of spin liquid state. In this system, the ordering of charges is suppressed completely because of the

geometrical frustration and, instead, a heavy-fermion metal with an effective electron mass of $100m_e$ is realized at low temperatures. [2]. A new mixed-valent spinel oxide $LiRh_2O_4$, a Rh-analogue of LiV_2O_4 , was discovered [3]. We found that, in contrast to LiV_2O_4 , an orbital ordering associated with cubic to tetragonal transition suppresses frustration and leads to a complex charge ordered state at low temperatures. This work was done in collaboration with Y.Okamoto, S.Niitaka, M.Nohara, H. Aruga-Katori, P.Jonson, S.Fujiyama and K.Kanoda

[1] Y. Okamoto et al., *Phys. Rev. Lett* 99, 137207 (2007).

[2] P. Jonson et al., *Phys. Rev. Lett.*99, 167402 (2007).

[3] Y. Okamoto et al., submitted.

Keywords: spinel, geometrical frustration, liquid state of spins and charges

MS.91.2

Acta Cryst. (2008). A64, C152

Local order and frustration in vanadate spinels

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Orbitally degenerate frustrated spinels, $Cd_{1-x}Zn_xV_2O_4$ were investigated using elastic and inelastic neutron scattering techniques. For the end members, $x = 0$ and 1, a tetragonal distortion is observed upon cooling through a Jahn-Teller coupling mechanism which leads to the formation of spin chains in the ab-plane. Upon further cooling, Neel ordering is established due to interchain coupling. In the doped compounds, bulk susceptibility shows that the macroscopic transitions to cooperative orbital ordering and long range antiferromagnetic ordering are absent. However, from the inelastic magnetic scattering measurements, it is suggested that the dynamic spin correlations at low temperatures have similar one dimensional characteristics as observed in the pure samples. The pair density function analysis of neutron diffraction data shows that the local atomic structure does not become random with doping but rather consists of two distinct environments corresponding to ZnV_2O_4 and CdV_2O_4 . This suggests that short-range orbital ordering is present which leads to the one dimensional character of the spin correlations even in the low temperature cubic phase of the doped compositions.

Keywords: local symmetry, one-dimensional, orbital degeneracy

MS.91.3

Acta Cryst. (2008). A64, C152-153

Controlling spin glass entropy - Frustrated magnetism in the spinels

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The zero point entropy of frustrated magnets is an interesting quantity, as it provides information on the degeneracy of their ground states. Indeed, much of the recent work on spin ices was triggered after the characterisation of their zero point entropies using specific

heat measurements. Spin glasses provide an important class of frustrated magnets. Typically based on disordered systems, they have found relevance in diverse areas of research, such as neural networks, the origin of life, and algorithm theory. Despite the theoretically prediction that these materials have a non-zero residual entropy, there have been no clear experimental studies of the entropy of a spin glass. This presentation describes an experimental study of the magnetic properties and zero point entropy of a series of $S=1/2$ spin glasses. Diamagnetic dilution in the spinel systems CuAl_2O_4 and CuGa_2O_4 forms isomorphic solid solutions $\text{Zn}_x\text{Cu}_{(1-x)}\text{Ga}_2\text{O}_4$ and $\text{Zn}_x\text{Cu}_{(1-x)}\text{Al}_2\text{O}_4$ that provides an opportunity to investigate the effect that non-magnetic substitution has on the spin glass properties of CuGa_2O_4 and on the entropy of the related spin glass states. Low temperature specific heat measurements were carried out on both CuGa_2O_4 and CuAl_2O_4 in order to determine the magnetic entropies, and compare them with the value theoretically predicted for $S = 1/2$ spin glasses. Both spinels were found to possess a non-zero magnetic entropy at 0K, with values that are significantly greater than the predicted value. These studies also indicate that the ground state degeneracy of these frustrated magnets can be controlled by chemical substitution.

Keywords: magnetic frustration, specific heat, magnetic ordering

MS.91.4

Acta Cryst. (2008). A64, C153

Polaronic behavior of Mn_4O_4 heterocubane clusters in LiMn_2O_4 spinel

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Crystals of LiMn_2O_4 undergo a structural phase transition near the room temperature. The high temperature (HT) form adopts a normal spinel-type structure (cubic, $Fd\bar{3}m$) with the octahedral sites populated statistically with heterovalent Mn^{III} and Mn^{IV} in the equal ratio. The low temperature (LT) form adopts a $3 \times 3 \times 1$ superstructure (orthorhombic, $Fddd$) with respect to the HT form, containing Mn^{III} , Mn^{IV} , and the intervalent Mn atoms. The synchrotron X-ray single-crystal electron-density analysis, carried out at the beamline 14A, Photon Factory, Tsukuba, revealed a large anisotropy of the atomic displacement parameters for part of O atoms, suggesting a possible occurrence of the bond-length fluctuation along the pseudo-tetragonal Jahn-Teller distortion parallel to the a-axis in the heterocubane Mn_4O_4 cluster. The cluster presumably shares three electrons among four e-parentage orbitals of Mn and behaves as a core of Zener-type polaron. The heterocubane Mn_4O_4 clusters are isolated from each other and embedded in an orbitally-ordered way in the charge-ordered matrix containing Mn^{III} and Mn^{IV} . The transition between the LT and HT forms of LiMn_2O_4 can thus be regarded as an order-disorder transition of the Zener-type heterocubane polarons.

Keywords: zener polaron, synchrotron X-ray diffraction, phase transition

MS.91.5

Acta Cryst. (2008). A64, C153

Magnetic structure of the quasi-one-dimensional, frustrated, spin-1 antiferromagnet CaV_2O_4

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We present the magnetic structure determination of the quasi-one-dimensional, frustrated, spin-1 chain material CaV_2O_4 by means of neutron diffraction. This material crystallizes in the post-spinel-type CaFe_2O_4 -type structure at room temperature (orthorhombic Pnam) and contains zig-zag chains of edge-sharing VO_6 octahedra along the crystallographic *c* direction. Nearest and next nearest neighbour V^{3+} -ions (spin-1) are almost equally spaced leading to competing antiferromagnetic exchange interactions and resulting in considerable geometrical frustration. The non-magnetic Ca^{2+} -ions act as spacers between the chains minimizing the interchain exchange coupling and making this system a low-dimensional quantum magnet. Upon cooling the material undergoes two phase transitions. A structural transition from orthorhombic to monoclinic occurs at $T_s=140\text{K}$. This distortion partially lifts the frustration of the system thus assisting the onset of long-range antiferromagnetic order below $T_N=71\text{K}$. By performing neutron diffraction experiments on CaV_2O_4 in the magnetically ordered phase, we found that it consists of two collinear antiferromagnetically coupled sub-chains, which are canted with respect to each other. The canting is a result of the distorted octahedral environment of the V^{3+} -ions, which lifts the orbital degeneracy of the Vanadium $3d^2$ electrons. Furthermore, the ordered magnetic moment of the V^{3+} -ions turned out to be is strongly suppressed, possibly due to strong quantum fluctuations caused by geometrical frustration and low-dimensional interactions. The analysis was challenging because the small monoclinic splitting resulted in twinned peaks whose intensity could only be separated by measuring a single crystal on a four-circle diffractometer.

Keywords: neutron diffraction, magnetic frustration, magnetic neutron scattering

MS.92.1

Acta Cryst. (2008). A64, C153–154

Federated repositories of X-ray diffraction images

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