MS38 P01

Effect of monovalent doping in the A site on structural and physical propeties of $La_{1-x}Ca_xMnO_3$ manganese oxides A. Cheikhrouhou[a,b], W. Cheikh-Rouhou Koubaa[a], A. Mehri[a], M. Koubaa[a], [a]Laboratoire de Physique des Matériaux, Faculté des Sciences de Sfax, B. P. 802, 3018 Sfax, Tunisia, [b]Laboratoire Louis NEEL, CNRS, B. P. 166, 38042 Grenoble Cedex 9, France.
E-mail: abdcheikhrouhou@yahoo.fr

Keywords: manganites, magnetoresistance, ferromagnetism,

The mixed valence perovskite manganese oxides $Ln_{1-x}M_xMnO_3$ where Ln is a rare earth element (Ln=La, Pr, Nd) and M is a divalent element (M=Sr, Ca, Ba, Pb) have been widely studied during the last decade in reason of their considerable interest owing to a colossal resistivity decrease in an applied magnetic field near the metal-insulator transition temperature. However only few studies have been performed on manganites where the bivalent element (Ca/Sr) has been partially substituted by monovalent element (Na, K, Ag). We studied the monovalent doping effect on the structural and physical properties of $La_{1-x}Ca_xMnO_3$ manganese oxides, we elaborated using the solid state reaction method $La_{1-x}Ca_{x-y}A_yMnO_3$ and $La_{1-x-y}A_yCa_xMnO_3$ samples with A=Na, K and Ag and x=0.35 and x=0.5 and studied their structural and physical properties and particularly the correlations between structure and physical properties. The parent compounds $La_{0.65}Ca_{0.35}MnO_3$ and $La_{0.5}Ca_{0.5}MnO_3$ have been chosen in reason of their physical properties; in fact $La_{0.65}Ca_{0.35}MnO_3$ compound exhibits a paramagnetic-ferromagnetic transition at T_C=265K while $La_{0.5}Ca_{0.5}MnO_3$ exhibits an antiferromagnetic charge order at about 175K.

MS38 P02

Deficiency effects on structure and physical properties in the A-site of $Pr_{1-x}Sr_xMnO_3$ manganese oxides with (x=0.2; 0.3; 0.4 and 0.5) W. Cheikh-Rouhou Koubaa[a], M. Koubaa[a], W. Boujelben[a], A. Cheikhrouhou[a,b] [a]Laboratoire de Physique des Matériaux, Faculté des Sciences de Sfax, B. P. 802, 3018 Sfax, Tunisia, [b]Laboratoire Louis NEEL, CNRS, B. P. 166, 38042 Grenoble Cedex 9, France.
E-mail: saissouma@yahoo.fr

Keywords: deficiency, ferromagnetism, manganites

We investigate the structural, magnetic and electrical properties of praseodymium and strontium deficient $Pr_{1-x-y}\square_ySr_xMnO_3$ and $Pr_{1-x}Sr_{x-y}\square_yMnO_3$ compounds with x=0.2, 0.3; 0.4 and 0.5 and 0<y<0.2. All our samples have been elaborated using the conventional solid state reaction at high temperature. Rietveld refinements of the X-ray diffraction patterns show that all our samples are single phase. The crystallographic structure depends strongly on the composition parent compound, the nature and the amount of the deficiency. For x=0.2 and x=0.3, praseodymium deficiencies lead to a reinforcing of the ferromagnetic-metallic behaviour at low temperature and an increase of the Curie temperature T_C while strontium deficiencies lead to a weakening of the ferromagnetic-metallic behaviour at low temperature and a decrease of the Curie temperature T_C. For x=0.4 and 0.5 the praseodymium and strontium deficiencies have not the same effects as for x=0.2 and x=0.3. The physical properties are strongly correlated to the crystallographic structure of our synthesized samples.

MS38 P03

Coexistence of the canted ferromagnetism and canted antiferromagnetism in $La_{0.6}Pr_{0.4}Mn_2Si_2$ Yalcin Elerman[a], Ilker Dincer[a], Helmut Ehrenberg,[b], Hartmut Fuess,[b] Gilles André[c], Ayhan Elmali[a] [a]Ankara University, Faculty of Engineering, Department of Engineering Physics, 06100 Besevler-Ankara Turkey, [b]Institute for Materials Science, Darmstadt University of Technology, Petersenstrasse 23 D-64287 Darmstadt Germany, [c]Laboratoire Léon Brillouin (CEA-CNRS), CEN-Saclay, 91191 Gif-Sur-Yvette, France
E-mail: elerman@ankara.edu.tr

Keywords: Neutron diffraction, Magnetic structures, Magnetic transitions

The magnetic structures of $La_{0.6}Pr_{0.4}Mn_2Si_2$ have been determined by the powder neutron diffraction between 1.5 and 308 K. According to magnetic measurements, this compound is antiferromagnetic below T_N^{inter}, ferromagnetic above T_N^{inter} up to T_C^{inter} and antiferromagnetic between T_C^{inter} and T_N^{intra}. The powder neutron diffraction results show that the magnetic structure is canted antiferromagnetic below 130 K and canted ferromagnetic between 240 and 297 K. The neutron diffraction patterns between 130 < T < 240 K indicate that the canted antiferromagnetic and ferromagnetic structure coexist. Since the magnetic moment values, the unit cell parameters and the scale parameters of the canted antiferromagnetism and canted ferromagnetism overlap at this temperature range, we use a special refinement procedure to refine the neutron diffraction patterns. Hofmann et al. [1] used a similar method to analyze the neutron diffraction patterns for $La_{0.8}Y_{0.2}Mn_2Si_2$. They assumed an identical canting angle for the canted antiferromagnetic and ferromagnetic structures. Because of the contraction on a and expansion on c, an identical canting angle for the antiferromagnetic and ferromagnetic structures is excluded. $La_{0.6}Pr_{0.4}Mn_2Si_2$ reveals a single ferromagnetic phase above 240 K, and the Rietveld refinements indicate different canting angles for the antiferromagnetic and ferromagnetic structures [2]. Therefore the model proposed in Ref. [1] is wrong. The spontaneous volume change and linear magnetostriction are derived. The maximum value of the spontaneous volume magnetostriction is about -0.37% at 50 K [2].

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MS38 P04

Maximal Subgroups of index ≤4 of Magnetic Groups D.B. Litvin, *Department of Physics, The Eberly College of Science, The Pennsylvania State University, Penn State Berks, P.O. Box 7009, Reading, PA 19610-6009, U.S.A.*
E-mail: u3c@psu.edu

Keywords: magnetic groups, subgroups, space groups

We have consider the one-, two-, and three-dimensional magnetic space groups and the two- and three-dimensional magnetic subperiodic groups, i.e. magnetic rod and magnetic layer groups. We have tabulated the

maximal subgroups of index ≤ 4 of a representative group of each type of magnetic group in the superfamilies of these groups.

MS38 P05

Magnetic structure of the Kagomé mixed compound $(Co_{0.5}Ni_{0.5})_3V_2O_8$ <u>N. Qureshi</u>,[a,b] H. Fuess,[a] H. Ehrenberg[c] B. Ouladdiaf,[b] T. C. Hansen,[b] Th. Wolf,[d] C. Meingast,[d] Q. Zhang,[d] W. Knafo,[d,e] H. v. Löhneysen[d,e] [a]*Institute for Materials Science, University of Technology, Darmstadt, Germany.* [b]*Institut Max von Laue-Paul Langevin, Grenoble, France.* [c]*Leibniz Institute for Solid State and Materials Research, Dresden, Germany.* [d]*Research Center Karlsruhe, Institute of Solid State Physics, Karlsruhe, Germany.* [e]*Physics Institute, Karlsruhe University, Karlsruhe, Germany.*
E-mail: <u>navidq@st.tu-darmstadt.de</u>

Keywords: magnetic structures, magnetic structure determination, neutron diffraction

$(Co_{0.5}Ni_{0.5})_3V_2O_8$ represents a mixed compound of the well investigated transition metal (M) orthooxovanadates $Ni_3V_2O_8$ (NVO) and $Co_3V_2O_8$ (CVO) labelled as Kagomé staircase structures, which are characterized by edge-sharing MO_6 octahedra isolated by nonmagnetic VO_4 tetrahedra. The crystallographic structure (orthorhombic space group Cmca) [1, 2] is interesting with respect to the magnetic properties as the magnetic ions form buckled planes of corner-sharing isosceles triangles representing an anisotropic variation of the ideal Kagomé net. Within these buckled planes, the Kagomé staircases, cross-tie ions on crystallographic (4a) sites link the linear chains of spine ions on (8e) sites. Due to the reduced symmetry of the Kagomé staircase geometry with respect to the ideal plane net the degree of frustration is lowered leading to interesting long range ordered magnetic structures. Magnetization and neutron diffraction experiments on a $(Co_{0.52}Ni_{0.48})_3V_2O_8$ powder sample [3] revealed only one magnetic phase transition into an antiferromagnetic ground state in contrast to the richness of magnetic phase transitions of its parent compounds [4, 5]. The magnetic structure is modulated by a composition dependent propagation vector $k=(\delta, 0, 0)$ with δ being 0.491(4) for $(Co_{0.52}Ni_{0.48})_3V_2O_8$ where a similarity to the NVO type magnetic structure was assumed [3]. Neutron single crystal diffraction experiments followed by group theory analysis produced a more detailed picture. The magnetic structure of $(Co_{0.5}Ni_{0.5})_3V_2O_8$ exhibits features, which differ from the predominantly collinear alignment of its parent compounds NVO and CVO, which exhibit a variety of magnetic structures with magnetic moments mainly oriented along the *a* axis [4-7]. The averaged magnetic moments of the statistically distributed Ni^{2+} and Co^{2+} ions are oriented in the *a-c* plane. They point either towards or away from the centers of the respective isosceles triangles of the Kagomé staircase structure if viewed as a projection along the *b* axis. The spin arrangement is close to a 120° configuration as expected for antiferromagnetically ordering systems on a Kagomé lattice. This result shows once again that the competition of the exchange interactions along various coupling pathways in this particular crystallographic system results in a variety of different interesting magnetic structures.

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MS38 P06

Magnetic structure of $Ba_7Co_6BrO_{17}$ <u>Pascal Roussel</u>, Matthieu Kauffmann, Olivier Mentré *UCCS CNRS UMR8181, Université de Lille, 59652 Villeneuve d'Ascq, France.* E-mail: <u>pascal.roussel@ensc-lille.fr</u>

Keywords: magnetic perovskite materials, neutron powder diffraction, new materials

At the basis of the search for original electronic and magnetic behaviour, a number of studies focus on the prospecting for new complex structural types within "hot" topics such as cobaltites (strong competition between magnetic ground states, attractive thermoelectricity, superconductivity …). In this context, we recently synthesized by solid state reaction the new $Ba_7Co_6BrO_{17}$ compound (P6$_3$/mmc: a=5.6611(1) Å and c=33.5672(8) Å) [1]. This cobaltite is built from a close-packing of [BaO$_3$] and [BaOBr] layers with a 14H stacking sequence (c'chhcc')$_2$, which creates Co_4O_{15} tetramers of face-sharing octahedra connected to their extremities to isolated tetrahedra by corner-sharing. This material is strongly related to the $12H-BaCoO_{2.6}$ [2] and $6H-Ba_6Co_6ClO_{16}$ [3] cobaltites, with the existence of common blocks. Measurement of the magnetic susceptibility χ against T has been performed under applied magnetic field of 1 T. The experiment reveals the existence of two transitions at 60 K and 30 K. The curve was fitted to the Curie-Weiss law in the paramagnetic domain (above 60 K), leading to the values p_{eff}=3.12 μB/Co and θ=55K This paramagnetic effective moment can be explained by assuming Co^{3+} S=1 and Co^{4+} S=3/2 i.e. cobalt atoms at the intermediate spin-state (considering the spin-only approximation). The positive θ value indicates important ferromagnetic exchanges among the structures. In order to understand the magnetic properties of this cobaltite, we collected neutron powder diffraction data on the G41 diffractometer (LLB Saclay, France). The pattern below 60 K revealed the onset of new reflections, this fact being ascribed to the occurrence of long-range magnetic ordering and confirming the magnetic transition previously reported. All those magnetic reflections were indexed in a commensurate lattice related to the crystallographic one by a propagation vector k=[000]. Among all the possible magnetic models, only those for which the exchange interactions between two tetrahedral cobalt orders antiferromagnetically went to convergence with acceptable reliability factors. The magnetic structure can be described as the antiferromagnetic coupling of ferromagnetic blocks (Co_4O_{15} + 2 CoO_4 units). This kind of magnetic structure has been previously reported for $6H-Ba_6Co_6ClO_{16}$ [4].

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