Keywords: neutron diffraction; polarized neutrons; X-ray magnetic circular dichroism

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Structural, Magnetic and Electric Properties of GaFe_{1-x}Mn_xO₃. <u>M.Bakr</u>^a, A. Senyshyn^a, H. Wang^a, G. Parzych^b, L.Dobrzynski^{b,c}, K.Szymański^c, H. Fuess^a. ^aInstitut for Materials Science, Darmstadt University of Technology, D - 64289 Darmstadt, Germany. ^bThe Soltan Institute for Nuclear Studies, Poland. ^cFaculty of Physics, University of Bialystok, Poland. E-mail: mbm1977@yahoo.com

Gallium iron oxide (GaFeO₂) is a member of a multiferroic family which exhibits ferrimagnetic and piezoelectric properties below room temperature [1-2]. This material has orthorhombic (double HCP Closed-Pack) crystal structure with space group P c 2_1 n with four different cation sites labeled Ga1, Ga2 (mostly occupied by gallium) and Fe1, Fe2 (mostly occupied by iron) [3-5]. The different physical properties of GaFeO₃ are strongly dependent on the distribution of cations within the structure. The magnetic properties of GaFeO₃ strongly depend on the preparation method which affects the cations distributed over different sites. Polycrystalline GaFe_{1-x}Mn_xO₃ materials have been prepared by a traditional solid state reaction (SR) and sol-gel (SG) methods. Structural analyses showed that the maximum Mn content is 10% and 50% for samples prepared by SR and SG, respectively. All samples crystallise in the orthorhombic system with P c 2, n space-group. The Curie temperature (T_c) for GaFeO₃ (SR) is about 190K and increases or reaches room temperature when the temperature of preparation is decreased from 1400°C to 700°C. The Curie temperature for SG reaction is slightly above room temperature. With increasing the Mn content the transition temperatures as well as the coercive field decrease. Dielectric investigations revealed a temperature independent anomaly at around 255 K with frequency dispersion of dielectric constant only for GaFeO₂ prepared at 700°C (SG) and Mn doped samples prepared by both methods. It follows from the neutron powder diffraction and Mössbauer spectroscopy revealed that GaFeO₂ exhibits a ferrimagnetic order with spins parallel to c-axis. Both, the cation and magnetic, orderings depend strongly on the preparation conditions.

[1] JP. Reimeka , *J. Appl.Phys.* 31 263S, **1960**, [2] E.A. Wood, *Acta Cryst.* 13, 682, **1960**, [3] S.C.Abrahams, J.M.Reddy and I.L.Bernstein, *Chem.Phy.*42, 3957-3968, **1965**, [4] G.T. Rado, *Phys. Rev.* Lett. 13, 335-337, **1964**, [5] T.Arima, D.Higashiyama, Y.Kaneko, J.P.He, T.Goto, S.Miyasaka, T.Kimura, K.Oikawa, T.Kamiyama, R.Kuumai, and Y.Tokura, *Phys.Rev.B* 70, 064426, 1-8, **2004**.

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Neutron Diffraction Study of DyVO₃ and HoVO₃. <u>Manfred Reehuis</u>^a, Clemens Ulrich^b, Jun Fujioka^c, Shigoki Miyasaka^c, Yoshinori Tokura^c, Bernhard

25th European Crystallographic Meeting, ECM 25, İstanbul, 2009 *Acta Cryst.* (2009). A**65**, s 69 Keimer^{b. a}Helmholtz-Zentrum Berlin, Germany. ^bMPI-Stuttgart, Germany. ^cUniversity of Tokyo, Japan. E-mail: <u>reehuis@helmholtz-berlin.de</u>

Vanadates with the formula RVO_2 (R = Y or rare-earth element) exhibit many exciting properties, which can be related to orbital or spin rearrangements [1], [2]. In order to provide a more complete basis for the theoretical description of the electronic properties of these compounds we have started to carry out a comprehensive investigation of the crystal and magnetic structures of YVO₂, NdVO₂ and TbVO, [3], [4]. In the room-temperature lattice structure the influence of the relative ionic sizes leads to tilts of the VO₆-octahedra. From La³⁺ to Lu³⁺ the distortions show a continuous increase due to the well-known lanthanide contraction. With decreasing temperature the vanadates show a structural phase transition at T_{s1} , where the orthorhombic structure (Pbnm) changes to a monoclinic structure with the space group $P2_1/b$ due to the onset of the cooperative Jahn-Teller effect and the onset of orbital ordering. In the monoclinic phase the magnetic moments of the $V^{\scriptscriptstyle 3\text{+}}\text{-}\text{ions}$ show antiferromagnetic ordering with the modes C_{y} , C_{y} and G_{z} , where the z-component is the weakest. A second structural phase transition (T_{s2}) could be observed for vanadates containing smaller R^{3+} -ions ($R^{3+} = Y^{3+}$, Ho³⁺ - Lu³⁺) [1]. Below T_{s2} the crystal structure changes back to the orthorhombic structure and the vanadium moments are purely G-type ordered along z [3], [4]. In DyVO₃, where the R^{3+} -ion is slightly larger than Ho³⁺, a critical phase competition between different spin-orbital-ordered states was observed only recently [5]. Our neutron diffraction experiments of DyVO3 showed that the transition to the pure G-type ordering sets in at $T_{s2} = 63(1)$ K. For YVO₃, where Y^{3+} is only slightly smaller than Dy^{3+} , this transition sets in at considerably higher temperature $T_{s2} = 77(1)$ K. As found earlier for YVO_3 the *G*-type ordering in $DyVO_3$ remains stable upon cooling from T_{s_2} down to 6 K. But with increasing temperature the monoclinic C-type phase surprisingly appears in DyVO, between 13 and 23 K. For HoVO₃ this intermediate phase could not be observed. On the other hand the second phase transition of this vanadate sets in (cooling process) at the strongly reduced temperature $T_{s_2} = 26(1)$. With increasing temperature it sets in at the higher value $T_{s_2} = 36(1)$ K, indicating the presence of strong hysteresis effects. Further it is important to note that both the magnetic moments of the Dy^{3+} and Ho^{3+} -ions show a long-range ferrimagnetic order up to the unusually high temperatures 23(1) K and 36(1) K, respectively. Our study clearly showed that strong exchange interactions between the magnetically ordered V-moments and the magnetic Dy³⁺- and Ho³⁺-ions lead to a reduction of the transition temperature T_{s_2} as well as to an increasing of the magnetic ordering temperature of the R^{3+} -ions.

Miyasaka S.; Okimoto Y.; Iwama M.; Tokura Y., *Phys. Rev. B*, **2003**, 68, 100406(R).
Blake G.R.; Palstra T.T.M.; Ren Y.; Nugroho A.A.; Menovsky A.A., *Phys. Rev. Lett.*, **2001**, 87, 245501.
Ulrich C.; Khaliullin G.; Sirker J.; Reehuis M.; Ohl M.; Miyasaka S.; Tokura Y.; Keimer B., Phys. Rev. Lett., **2003**, 91, 257202.
Reehuis M.; Ulrich C.; Pattison P.; Ouladdiaf B.; Rheinstädter M.C.; Ohl M.; Regnault L.P.; Miyasaka S.; Tokura

Y.; Keimer B., *Phys. Rev. B*, **2006**, 73, 094440. [5] Miyasaka S.; Yasue T.; Fujioka J.; Yamasaki Y.; Okimoto Y.; Kumai R.; Arima T.; Tokura Y., Phys. Rev. Lett., **2007**, 99, 217201.

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