s14.m39.o3 **Crystal and magnetic order in nanosized transition-metal oxides**. K. Krezhov[1], E. Sváb[2], Gy. Mészáros[2], F. Bourée[3], Z. Somogyvári[2], P. Konstantinov[1], I. Nedkov[4], [1]*Institute for Nuclear Research and Nuclear Energy, 72 Tzarigradsko Chaussee, BU-1784 Sofia, Bulgaria* [2]*Research Institute for Solid State Physics and Optics, 1525 Budapest, POB 49, Hungary,* [3]*Laboratoire Léon Brillouin, CEA/Saclay, 91191 Gif-sur-Yvette, France,* [4]*Institute of Electronics, 72 Tzarigradsko Chaussee, BU-1784 Sofia, Bulgaria. E-mail: krezhova@stil.acad.bg*

Keywords: Powder diffraction; Cation distribution; Nanoparticles

Revolutionary consequences for science and technology are expected to follow the deeper understanding and control of the structure signatures of condensed matter at the nanometric scale. This study, combining mainly results from Rietveld refinement of neutron and X-ray powder data with findings by other techniques, is focussed on the structure of nanosized ferroxides (magnetite, maghemite, M-type substituted barium hexaferrite) and nickel cobaltites prepared by soft chemistry methods. For Bragg scattering the interparticle interference is of no relevance and size, surface and shape effects' structural impact is tracked down through evidence for changing local symmetry, interatomic distances, cation distribution and sublattice magnetic moment compared with bulk material. The known preference of Ni^{2+} ions to occupy octahedral spinel sites is confirmed in $Ni_xCo_{3-x}O_4$ (Fd-3m, 15 nm average size, $0<x<1$, six compositions) but a small fraction of tetrahedrally coordinated nickel is established as well. The nearly linear dependence on composition found for the Ni-occupancy per tetrahedral site extrapolates to 0.1 for the presumably normal spinel $NiCo_2O_4$ (x=1). Effects implying a predominant volume expansion of the tetrahedral voids come out in Fe_3O_4 with a grain size increasing from 17 to 640 nm as determined by modified Williamson-Hall plots. In acicular nanoparticles of maghemite (γ-Fe_2O_3) the determined distribution and ordering of vacancies is associated with formation of a tripled unit cell of lower symmetry ($P4_12_12$ specified) even at the size of 240×30 nm. For $BaFe_{12-2x}(CoTi)_xO_{19}$ ($P6_3/mmc$, x=0.45-0.85) the evidence for higher thermal expansion anisotropy, reduction of sublattice magnetic moments, and short-ranged magnetic noncollinearity manifested by diffuse scattering, is related to grain-size and (Co^{2+}, Ti^{4+}) distribution effects on the coordination polyhedra. Preliminary results at different stages of the study were reported in the papers listed below.

The partial financial support under contracts OTKA-T42495 and BG-NFSR-F1202 is acknowledged.

[1] Krezhov, K., Konstantinov, P., Svab, E., & Meszaros, Gy. (2000) *Mater. Sci. Forum* 321- 324, 785-790.
[2] Somogyvari, Z., Svab, E., Meszaros, Gy., Krezhov, K., Konstantinov, P., Ungar, T. & Gubicza, J. (2001), *Mater. Sci. Forum* 378- 381, 771-776.
[3] Somogyvari, Z., Svab, E., Meszaros, Gy., Krezhov, K., Konstantinov, P., Nedkov, I. & Bouree, F. (2002) *J. Appl. Phys*. **91**, 6185-6187.
[4] Krezhov, K., Somogyvari, Z., Meszaros, Gy., Svab, E., Nedkov, I. & Bouree, F. *(2002) Appl. Phys.* A**74** [Suppl.] S 1086- S 1089.
[5] Somogyvari, Z., Svab, E., Meszaros, Gy., Krezhov, K., Nedkov, I., Sajo, I. & Bouree, F. (2002) *Appl. Phys*. A**74**, S1077-S1079.

s14.m39.o4 **Advanced Analysis of Neutron Total Scattering Data: Modelling Disorder in Network Structures.** David A Keen[a], Martin T Dove[b] and Matt G Tucker[b], [a]*Department of Physics, University of Oxford, Clarendon Laboratory, Parks Road, Oxford OX1 3PU U.K. and ISIS Facility, Rutherford Appleton Laboratory, Didcot, Oxon OX11 0QX U.K.,* [b]*Department of Earth Sciences, University of Cambridge, Downing Street, Cambridge CB2 3EQ U.K. E-mail: d.keen1@physics.ox.ac.uk*

Keywords: Neutron Diffraction; RMC; Structural Disorder

Total scattering data from the advanced neutron powder diffractometer, GEM, at ISIS have been used to quantitatively characterise the disorder present in network materials. Here we describe the unique characteristics of the instrumentation, the reverse Monte Carlo method of data analysis and show results from a number of different systems. These results are used to characterise the local disorder in the α-β phase transition in quartz, the low-temperature phase transition in $SrTiO_3$, and the local origin of negative thermal expansion in ZrW_2O_8.