

0.02 and 0.06) alloys are found $-16.5 \text{ J.kg}^{-1}\text{K}^{-1}$ and $-14.2 \text{ J.kg}^{-1}\text{K}^{-1}$ from the DSC analysis at around the structural transition temperatures, respectively. Since the values of the relative cooling power and the isothermal magnetic entropy change of the $x=0.02$ alloy is bigger than of the $\text{Gd}_5\text{Ge}_{2.05}\text{Si}_{1.95}$ alloy, this alloy should be good candidate for room temperature magnetic cooling technology [2].

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Opechowski-Guccione-like symbols of magnetic space groups. Hans Grimmer, *Laboratory for Developments and Methods, Research with Neutrons and Muons, Paul Scherrer Institut, Villigen, Switzerland*
E-mail: Hans.Grimmer@psi.ch

For the magnetic space group types with black and white lattice two sets of symbols have been proposed: the BNS symbols [1] and the OG symbols [2]. Whereas generators of the group can be read off the BNS symbol, the International Tables for X-Ray Crystallography (1952) must be consulted to interpret the OG symbols in the cases where the black and white lattice is centred. We shall define OG-like symbols in the case of centred lattices in such a way that generators of the group can be deduced directly from the symbol [3]. The definition generalizes a proposal of Bertaut [4] for crystal class *mmm* to every crystal class.

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FA5-MS41-P07

Temperature dependent Neutron Diffraction Studies on Iron Pnictide Single Crystals Martin Meven^a, Yixi Su^b, Y. Xiao^c, ^aFRM II, *Technische Universität München, Germany*, ^bJCNS, *IFF, Forschungszentrum Jülich, Outstation at FRM II, Garching, Germany*, ^cIFF, *Forschungszentrum Juelich, Germany*
E-mail: martin.meven@frm2.tum.de

The single crystal diffractometer (SCD) HEiDi at the hot source of the research neutron source Heinz Maier-Leibnitz (FRM II) was developed as a co-operation of the RWTH Aachen and the TU München [1]. The short neutron wavelengths ($0.4 \text{ \AA} < \lambda < 1.2 \text{ \AA}$) of the instrument allow detailed studies of nuclear structures and the magnetic order of compounds with similar or highly absorbing elements. Thus, HEiDi is an ideal tool for studies on the recently discovered superconducting iron pnictides. In spite of the different chemical composition there are significant similarities between the iron pnictides and the high- T_c

cuprates discovered in 1986. In both cases the layered structures undergo a crystallographic phase transition from a tetragonal room/high temperature phase to an orthorhombic low temperature phase. In addition, doping with suitable elements influences the appearance and disappearance of magnetic and superconducting phases significantly.

Detailed studies of undoped single crystals of BaFe_2As_2 and EuFe_2As_2 were performed on the SCD HEiDi to improve the understanding of the superconducting A-122 compounds. Due to the combination of platelike sample shapes, the complexity of the orthorhombic phase (reflection splitting due to appearance of domains and twinning) and the high absorption of the Eu sample made the precise data collections as well as the accurate interpretation of the results quite challenging but gave a deep insight to the phase transitions and magnetic order at low temperatures [2, 3] of these compounds.

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FA5-MS41-P10

Structural Aspect of Stabilization of Magnetic Particles in Solution: SAXS Study Eleonora Shtykova^a, Petr Konarev^b, Lyudmila Bronstein^c, Dmitri Svergun^b, ^a*Institute of Crystallography, Russian Academy of Sciences, Moscow, Russia*, ^bEMBL Hamburg Outstation, Germany, ^c*Indiana University, Department of Chemistry, USA*
E-mail: viwopix@yahoo.co.uk

A problem of stabilization of iron oxide magnetic nanoparticles (NPs) in solution is of special importance due to their possible application in life science, medicine, and particularly in anti-cancer therapy. Precondition for such applications is water solubility, which can be achieved by introducing a biocompatible shell on the hydrophobic NP surface. These coatings must fulfill certain requirements, and, first of all, they must prevent the aggregation of nanoparticles in solution. Functional properties of the protective shells depend strongly on their thickness, density, chemical composition and structure. Moreover, the practical use of the ferromagnetic liquids is determined by the metal particle shapes, size and size distributions. Therefore, all these characteristics of the specimens should be comprehensively characterized. In this work we report structure and properties of iron oxide NPs synthesized by decomposition of iron oleates and encapsulated by different methods. We analyze also the process of micellization of differently grafted PMAcOD in water solution, and the ability of the various coatings to encapsulate the NPs. The detailed structural investigation of the specimens was performed using small angle X-ray scattering (SAXS) and a complex of modern tools of SAXS data interpretation and modeling.

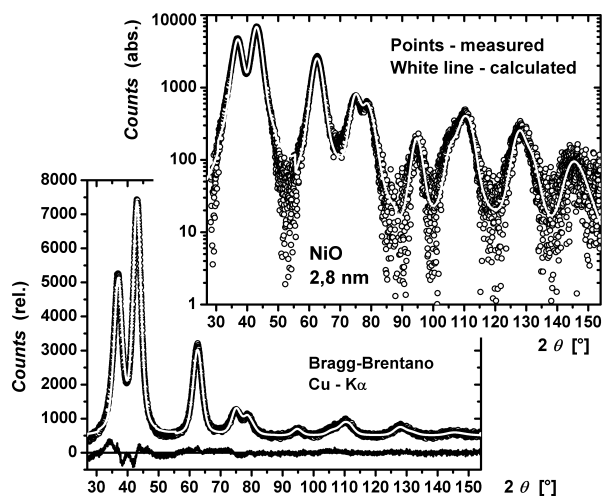
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Keywords: small-angle X-ray scattering, structure determination, computer modeling

FA5-MS41-P11

Structure-Magnetism Correlations in *nc*-NiO: High-Sensitivity Powder Diffraction. Marek Petrik^a, Bernd Harbrecht^a, ^a*Department of Chemistry and Center of Materials Science, Philipps University Marburg, Germany*
E-mail: petrik@chemie.uni-marburg.de

Nickel oxide NiO is a robust room-temperature antiferromagnet, distinguished by strong super-exchange interactions (Néel temperature $T_N = 523$ K) and a simple magnetic (*fcc*-based type II) and atomic (NaCl-type above T_N) structure. This has made NiO the model antiferromagnet of choice for over half a century. In the last two decades, renewed interest arose in the marked ferrimagnetism observed in nanocrystalline (*nc*-) NiO (Richardson's phenomenon).^[1] Recently, we demonstrated that this anomalous nanomagnetism may be explained by a Néel-type random spin-sublattice occupation.^[2] The next step is to find an explanation for the unusual size-dependent magnetic anisotropy modulation in *nc*-NiO.^[3] To this end, the lattice distortions in NiO nanocrystals have been re-examined by high-sensitivity x-ray powder diffraction, employing a latest-generation semiconductor array detector. Powder patterns of nanocrystals from 1.8 nm through the whole mesoscopic range up to 50 nm have been consistently refined using a basic set of Rietveld parameters (including overall *B* isotropic).



The quality of the fits even at high 2θ (note the semi-logarithmic scale in the upper figure) indicates that, unlike other ultra-fine nanoparticles (e.g. CdSe), NiO remains structurally intact, without faulting or major surface reconstruction, even on the ultra-nanoscale. However, two remarkable changes emerge at the lower end of the mesoscale (viz. for 2 to 8 nm NiO crystallites): the Rietveld refinements indicate (1) a significantly enhanced antiferromagnetic exchange striction (rhombohedral contraction),^[3] up to 20 times larger than in the bulk, and (2) below 5 nm, a surplus random atomic displacement of up to 2,3(3) Å² (static, non-thermal, as evidenced by the unaltered Debye temperature calculated from IR spectra). These phenomena correlate with the above mentioned anomalous modulation – as a function of size – of the magnetocrystalline anisotropy (obtained for the first time^[3] from Néel-Wohlfarth and

Langevin plots of DC magnetisation data) and point towards an explanation for this novel finite-size effect.

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