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The magneto-structural transformation materials, which experience the crystallographic and magnetic phase transition simultaneously, have attracted considerable attention not only for their importance in fundamental physics but also for their promising applications as multifunctional materials. Magnetic refrigeration based on the magnetocaloric effect (MCE) is a possible alternative to the current vapor compression technology [1]. Nowadays, most studies on magnetic refrigerants are focused on materials undergoing a first order phase transition because of their potential applications at room temperature.

The $CoMnGe_{0.95}Ga_{0.05}$ compound was prepared by arc melting by using high-purity elements. Synchrotron experiments were performed in the temperature range between 290 and 390 K on B2 in HASYLAB/DESY in Hamburg. A synchrotron X-ray wavelength of 0.688105 Å was used. Magnetic measurements were performed as functions of temperature and magnetic fields with Physical Properties Measurements System-PPMS between 5 and 350 K under magnetic field up to 7 Tesla.

Synchrotron experiments shows that this compound exhibits the structural transition from high temperature phase (orthorhombic-space group: Pnma) to low temperature phase (cubic-space group: $P6_3/mmc$) around the room temperature. According to Rietveld refinement, the unit cell volume of the high temperature phase is 77.3 $Å^3$ and the unit cell volume of low temperature phase is 160.9 $Å^3$ at 300 K.

According to temperature dependence of magnetization measurements, this compound has thermal hysteresis between FC and FH curves and this thermal hysteresis confirms the structural transition around T_C. While on FC mode the Curie temperature is 308 K, the Curie temperature is 319 K on FH mode. According to M(H) curves, this compound exhibit magnetic field induced structural transition. This magneto-structural transition makes this material very important for magnetic cooling technology. The magnetocaloric effect of this compound is estimated by using Maxwell equation. The magnetic entropy change is 4.5 J/kg.K and 30.9 J/kg.K for the magnetic field change of 1 Tesla and 7 Tesla, respectively.

This work was supported by The Scientific and Technological Research Council of Turkey-TÜBİTAK (Project Number: 109T743).

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Keywords: synchrotron experiments, magneto-structural transition, magnetic measurements

MS96.P06

Acta Cryst. (2011) A**67,** C802

Magnetic space groups: database and extinction rules for magnetic diffraction

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Based on the recent compilations of magnetic space groups [1,2], a Magnetic Space Groups Database has been developed. This database is freely available on the Bilbao Crystallographic Server (www.cryst.ehu.es) [3], and includes useful data such as general positions (symmetry operations in matrix form), special Wyckoff positions, etc. Using this database and in order to facilitate the systematic use of extinction rules in magnetic non-polarized neutron diffraction analysis of magnetic structures, we have developed the computer tool MAGNEXT that is also freely available on the Bilbao Crystallographic Server. The derivation of the extinction rules for magnetic diffraction is somewhat more complex compared with that of non-magnetic diffraction because of the axial vector character of the magnetic structure factor and its different and more complicated relation to the intensity. In fact, there are no listings of magnetic diffraction extinction rules comparable to those available for non-magnetic diffraction. This program is a contribution for changing this situation. MAGNEXT provides the extinction rules for non-polarized neutron diffraction corresponding to any Shubnikov magnetic space group. Illustrative examples are provided to demonstrate the utility of the program. Although not having the strong resolving power of the extinction rules of conventional non-magnetic crystallography, the extinction rules for magnetic diffraction can be useful for the systematic analysis and determination of magnetic structures, since they may facilitate the identification of their magnetic space group.

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Keywords: extinctions, magnetic symmetry, Bilbao crystallographic server

MS96.P07

Acta Cryst. (2011) A**67,** C802-C803

Magnetic structures of the family $R_mM_nIn_{3m+2n}$ of intermetallic compounds

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The family $R_mM_nIn_{3m+2n}$ (R = Ce - Tb; M = Rh, Ir or Co; m = 1, 2; n = 0, 1) has been intensively investigated because its close relationship with the interesting physical properties found in other compounds of this family, specially for the R = Ce compounds, for whose a heavy fermion behavior with unconventional superconductivity (USC) has been reported. [1,2]

In this work we present a systematic study of the physical properties and the determination of magnetic structures of a new series of isostructural compounds $R_mM_nIn_{3m+2n}$ (R = Gd, Tb, Sm; M = Rh, Ir; m = 1, 2; n = 0, 1) exploring their relationship with physical properties of Ce-based compounds from this family. The magnetic structures of tetragonal Gd_2IrIn_8, $GdRhIn_5$, $TbRhIn_5$, Tb_2RhIn_8, Sm_2IrIn_8 and cubic $GdIn_3$ compounds have been determined using x-ray magnetic scattering (XRMS) at the bending magnet XRD2 beamline of the Laboratório Nacional de Luz Síncrotron (LNLS), in Campinas, Brazil. All these systems order antiferromagnetically in commensurate structures below their Nèel temperatures (T_N) with propagation vectors (1/2,0,0), (0,1/2,1/2), (1/2,0,1/2), (1/2,1/2,1/2), (1/2,0,0) and (1/2,1/2,0), respectively [3-6]. The comparison between all the determined magnetic structures will be performed in terms of crystal field (CEF) effects along the series. The magnetic moments of rare earth ions are oriented in the tetragonal *ab*-plane for R = Gd and Sm_2IrIn_8 compounds, while for the Tb-based systems order along the *c*-axis direction. T_N is increased along the tetragonal Tb-based compounds (Tb1-1-5 and Tb2-1-8) when compared to the cubic $TbIn_3$ compound ($T_N \sim 32$ K), as has been found for Nd-based compounds from this family [7].

On the other hand, neutron diffraction experiments have been performed in the La- and Y-doped $TbRhIn_5$ intermetallics in the AFM ordered phase (at the dilution limit of 40% of doping) at the Echidna (HRPD) instrument of the OPAL reactor, Australia. Our results show that there are no change in the magnetic moments orientation when compared to the non-doped compound (along tetragonal c-axis), the propagation vector remains the same and the size of the Tb moment is approximately the expected for a single Tb^{3+} ion.

We will discuss the details of magnetic structures determination as a function of CEF effects and how they are responsible in determining the magnetic moment directions for different *R* ions from this series as well as in determining the T_N evolution along the series and the behavior of magnetic susceptibility and specific heat.

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Keywords: diffraction, magnetism, synchrotron

MS96.P08

Acta Cryst. (2011) A**67,** C803

Structural biology and SAXS beamlines at the photon factory

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The Photon Factory (PF) is currently operating five structural biology beamlines, BL-1A, BL-5A, BL-17A, NW12A, NE3A, and two SAXS beamlines, BL-10C and BL-15A. Whereas all the structural biology beamlines use insertion device sources, the SAXS beamlines are conventional bending magnet sources.

BL-5A, NW12A and NE3A are high-throuput beamlines and we facilitate automation of the beamline operation with developments of sample exchange robots PAM, automated sample centering system and unified beamline control software [1,2]. Recently we started fully-automated data collection operation and it has been well used by the pharmaceutical companies.

BL-1A and BL-17A are small focus beamlines, dedicated to the micro crystal structure determination. In addition, softer xrays, 4 keV (BL-1A) and 6 keV (BL-17A), are available for low energy SAD structure analysis. We are now developing the helium chamber system to reduce the background.

BL-10C and BL-15A are two of the oldest beamlines at the PF and we have started upgrades of the SAXS beamlines [3]. We installed a 2-dimentional detector, RIGAKU R-AXIS 7 at BL-10C for the experiments of liquid samples. At BL-15A, we installed a flat panel detector, Hamamatsu C9728DK-10 for WAXS exeriments. We have a plan to construct a new insertion device SAXS beamline at BL-15A. We will move the current BL-15A to BL-6A this summer and will develop a new BL-15A beamline for SAXS experiments using small focus and softer energy x-rays.

We will present current status of the beamline upgrades and our future plans.

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Keywords: synchrotron, crystallography, SAXS

MS96.P09

Acta Cryst. (2011) A**67,** C803

Magnetic dynamical structures of possible spin-peierls system TiOBr

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Newly proposed spin-Peierls system Ti*OX* (*X*: Cl, Br) has been revealed showing exotic structural and magnetic properties such as a successive phase transition, one-dimensional (1D) nature associated with orbital ordering of Ti ions and super-lattice structure being related to the Peierls instability [1-5]. It is pointed out that resulting only from an arrangement of Ti d_{xy} orbital, the formation of 1D spin chains and the spin-Peierls transition will be realized. Recently, it has been demonstrated that TiOBr also exhibits two successive phase transitions similar to TiOCl at T_{c1}=27K and T_{c2}=47K. Here we carried out inelastic neutron experiments in order to find the evidence of spin-Peierls transition. The inelastic spectrum with a large amount of poly crystalline sample of TiOBr shows the localized signal in the vicinity of the magnetic zone center Q=0.9Å^{-1}. Observed spin gap like signal lies at energy of ΔE~10meV. The gap energy in TiOBr is expected much higher from measured thermodynamic properties and by analogy with TiOCl. Constant Q cuts of the observed $S(Q,E)$ map show some Q-dependent structure in its intensity indicating the signal is sample oriented. The Q structure quite reveals the intensity is well explained by the powder averaged dynamical structure.

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Keywords: 1D, magnetism, dynamics

MS97.P01

Acta Cryst. (2011) A**67,** C803-C804

Making crystallography appealing to secondary school students

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Science has been established as a critical part of the secondary school curricula. Sadly, Crystallography is often left out of the teaching curricula for students at secondary school. Educators usually assume that teaching crystallography requires advanced science knowledge and that X-ray instruments are insecure, inaccessible, unsafe or difficult to use.