

KEK-PF and BL08W of SPring-8, respectively. EPMA analysis was made at Center for Material Research by Instrumental Analysis in Gunma University.

The spin and orbital magnetic form factors of $\text{Pd}_{3.2}\text{Co}_{0.8}$ and Fe_3Pt were measured by the XMD for nearly twenty reciprocal lattice points, and the magnetic Compton profile (MCP) of $\text{Pd}_{3.2}\text{Co}_{0.8}$ was obtained for three directions along the principal axes [100], [110] and [111].

The observed spin and orbital magnetic form factors were fitted with atomic-model theoretical form factors based on the dipole approximation in order to obtain the spin and orbital magnetic moment of each constituent atom of the alloys. Theoretical form factors for 3d elements of Co and Fe and 4d element of Pd were quoted from the literature [1]. Those for 5d element of Pt were calculated by the authors (K.K. & T.N.) as they were not presented in literatures. The observed MCPs have provided information about the spin moment and directional anisotropy of the momentum distribution of electrons with spin.

The experimental results are as follows. (1) Sum of the spin and orbital moment of $\text{Pd}_{3.2}\text{Co}_{0.8}$ by the XMD ($2.3\mu_B$ and $0.8\mu_B$, respectively) is $3.1\mu_B$, which is consistent with the magnetic moment $3.16\mu_B$ observed by the magnetization measurement. (2) The estimated spin moment of $\text{Pd}_{3.2}\text{Co}_{0.8}$ by the MCP is $2.36\mu_B$ which is in agreement with that of the above XMD result. (3) For Fe_3Pt the orbital moment is almost quenched and the spin moment is $6.8\mu_B$ which is corresponding to the value $6.68\mu_B$ by the magnetization measurement. (4) Directional anisotropy is observed for the three MCPs of $\text{Pd}_{3.2}\text{Co}_{0.8}$. These results are compared with the other experimental results such as polarized neutron diffraction [2] and the MCS. [3,4]

[1] B.J. Brown, *International Tables for Crystallography Vol. C* (Eds, A.J.C. Wilson and E. Prince, Kluwer Academic Publishers) **1999**, 450-457. [2] Y. Ito, T. Mizoguchi, *Solid State Commun.* **1974**, *15*, 807-809. [3] J.W. Taylor, J.A. Duffy, J. Poulter, A.M. Bebb, M.J. Cooper, J.E. McCarthy, D.N. Timms, J.B. Staunton, F. Itoh, H. Sakurai, B.L. Ahuja, *Phys. Rev. B* **2001**, *65*, 024442 1-7. [4] J.W. Taylor, J.A. Duffy, A.M. Bebb, J.E. McCarthy, M.R. Lees, M.J. Cooper, D. N. Timms, *Phys. Rev. B* **2002**, *65*, 224408 1-8.

Keywords: X-ray_magnetic_diffraction, magnetic_compton_scattering, metallic alloy

MS48.P05

Acta Cryst. (2011) A67, C531

Perpendicular magnetic anisotropy in Co/Pd multilayer grown by MBE technique

Kosuke Suzuki,^a Naoto Go,^a Shun Emoto,^a Masayoshi Itou,^b Yoshiharu Sakurai,^b Hiroshi Sakurai,^a ^aDepartment of Production Science and Technology, Gunma University, Gunma (Japan). ^bJapan Synchrotron Radiation Research Institute, SPring-8, Hyogo (Japan). E-mail: kosuzuki@gunma-u.ac.jp

Since discovery of high perpendicular magnetic anisotropy (PMA) in Co/Pd multilayer [1], they have attracted much attention for application to high density magnetic recording media. In order to achieve the high density recording, it is important to control the PMA energy in Co/Pd multilayer. It has been reported that the PMA energy in the Co/Pd multilayer depend on Pd layer thickness [2,3]. However the origin of these phenomena is unclear. The interface of the multilayer may affect the PMA energy. In this study we compare the two Co/Pd multilayers with smooth and rough interface.

A Co(1.5nm)/Pd(2.6nm) multilayer was grown on SiN membrane substrate by using effusion-cell of MBE technique. The deposition temperatures of Co and Pd were 1515°C and 1405°C, respectively. Deposition rates of Co and Pd were 0.5nm/min and 2nm/min, respectively. The XRD measurement showed fcc(111) texture and

satellite peaks. The satellite peaks confirm the smooth interface.

The Co(1.6nm)/Pd(4.0nm) multilayer was grown by sputter technique previously [4]. The XRD measurement showed fcc(111) texture. Smaller satellite peak intensities suggest rougher interface than multilayer by the MBE.

Magnetization measurement showed that the PMA energy of the Co(1.5nm)/Pd(2.6nm) multilayer was $1.15 \times 10^6 \text{erg/cc}$, and the Co(1.6nm)/Pd(4.0nm) multilayer was $1.2 \times 10^6 \text{erg/cc}$. Two multilayers have almost the same PMA energy, even if the Co(1.5nm)/Pd(2.6nm) multilayer with the smooth interface has thinner Pd layer thickness.

In order to measure the shape of wave function in the two multilayers, magnetic Compton profiles (MCPs) were measured on BL08W of the SPring-8. Figure 1 shows MCPs for the Co(1.5nm)/Pd(2.6nm) multilayer and Co(1.6nm)/Pd(4.0nm) multilayer. Both the MCPs are almost the same and it is suggested that wave function for the two multilayers are almost the same.

In conclusion we successfully control wave function and adjust the PMA energy by controlling the interface in Co/Pd multilayer.

[1] P.F. Garcia, A.D. Meinhardt, A. Suna: *Appl. Phys. Lett.* **1985**, *47* 178-180. [2] H. Nemoto, Y. Hosoe: *J. Appl. Phys.* **2005**, *97*, 10J109 [3] P.F. Garcia: *J. Appl. Phys.* **1988**, *63*, 5066. [4] M.Ota: Gunma University master thesis **2006**, in Japanese.

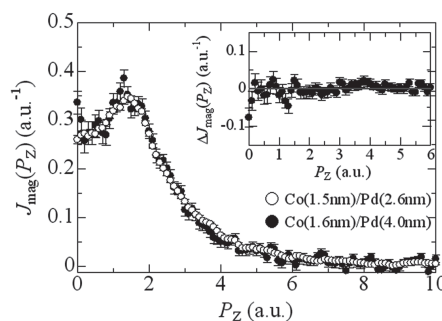


Fig.1 Magnetic Compton profiles (MCPs) of Co(1.5nm)/Pd(2.6nm) (open circles) and Co(1.6nm)/Pd(4.0nm) (solid circles) multilayers. The inset shows difference of the MCPs.

Keywords: multilayer, magnetic_compton_profile, magnetic_anisotropy

MS49.P01

Acta Cryst. (2011) A67, C531-C532

Growth and characterization of selectively doped surface modified ZnO nanocrystals

K. Byrappa,^a K. Namratha,^a D. Ehrentraut,^b G.K.L. Goh,^c T. Adschiri,^d ^aCrystal Growth and Materials Science Laboratory, University of Mysore, Manasagangothri, (India). ^bWorld Premier International Research Center - Advanced Institute for Materials Research (WPI-AIMR), Tohoku University, (Japan), ^cInstitute of Materials Research and Engineering, Agency for Science, Technology and Research, (Singapore). ^dInstitute of Multidisciplinary Research for Advanced Materials, Tohoku University, (Japan). Email: kbyrappa@gmail.com

ZnO nanocrystals find extensive application potential in modern technology for the fabrication of UV- diode laser and ZnO light emitting structures because of its wide and direct bandgap (3.37 eV) and with a large exciton binding energy (60 meV). ZnO has already been widely used in piezoelectric transducers, gas sensors, optical wave guides, transparent conductive films, varistors, solar cell windows, bulk acoustic wave devices, heterogeneous photocatalyst, etc. There are several methods employed popularly in the synthesis of ZnO nanocrystals. However, the hydrothermal method has been proved to be the most

favourable method due to homogenous or heterogeneous chemical reaction through a highly controlled diffusion leading to the formation of high quality nanocrystals having desired size, shape, dispersability and properties. Several approaches have been adopted by researchers to control size, shape, dispersability and in turn the properties of materials. Amongst them selective doping, precursors used, surfactants, synthesis method, etc. are important ones. Surfactants also help in modifying the surface charge of nanocrystals, such that, the material becomes either hydrophobic or hydrophilic. Experiments were carried out at 150°C with autogeneous pressure over an experimental duration of 16 hours in General Purpose autoclaves provided with Teflon liners. A variety of organic and inorganic solvents (propanol, ethanol, HCl, NaOH, HF) and also various surface modifiers (oleic acid, gluconic acid, *n*-butylamine, hexaldehyde, and benzylaldehyde) were tried. ZnO was selectively doped with molybdenum, silver, niobium, and also co-doping with silver and chromium has been carried out. The products were freeze dried and subjected to a systematic characterization using powder XRD, FTIR, UV-Vis spectroscopy, Thermal analysis, SEM, TEM, and Photoluminescence spectroscopy. The powder x-ray data shows homogeneous resultant product with high crystallinity. The FTIR spectra show the presence of various functional groups depending upon the type of surface modifier used in the *in situ* surface modification. TGA curves show the release of hydroxyl, carbonates and other organic molecules up to 500°C. UV-VIS spectroscopy study indicates the shift in the band gap depending upon the doping metal(s) and the band gap also shifts slightly accordingly. Photoluminescence spectra of pure and doped and surface modified ZnO nanocrystals show very interesting results which well correlates with the powder XRD and photocatalytic data. Higher concentration of dopants leads to structural distortion and contributes to the worsening of photocatalytic properties as well as lowering free exciton energy peaks. The application potential of products was evaluated using photocatalytic degradation of organic dyes and the ZnO nanocrystals synthesized are highly effective for the degradation of several toxic organic dyes.

[1] K. Namratha, M.B. Nayan, K. Byrappa, *Mater. Res. Innovat.* **2011**, *15*, DOS 10.1179/14330751x12922272563743. [2] K. Byrappa, K. Namratha, *Prog. Cryst. Growth Charact. Mater.* **2011** (in print).

Keywords: In situ surface modification, hydrothermal and solvothermal synthesis, photocatalysis.

MS49.P02

Acta Cryst. (2011) **A67**, C532

Growth of metal oxide – Organic hybrid nanocrystals and their interfaces in environmental applications

K. Byrappa, K. Namratha, *Crystal Growth and Materials Science Laboratory, P.B. No.21, University of Mysore, Manasagangothri, Mysore 570006, (India)*. Email: kbyrappa@gmail.com

Metal oxides, particularly TiO₂ and ZnO find extensive applications in modern technology including photocatalysis for environmental issues. Major breakthrough occurred during 1970s when Fujishima and Honda (1972) reported electrochemical photolysis of water at semiconductor electrode (TiO₂) [1]. With the discovery of quantization effect during the late 1970s, the size reduction in metal oxide semiconductors became a major objective to achieve higher efficiency in their applications. Difficulties in the growth of metal oxide nanocrystals were associated with the control of size, morphology, coagulation, reproducibility of results and dispersability. During 1990s several such attempts were made on the use of organic molecules as ligands or capping agents or surfactants. Also *ex situ* surface modification was tried with limited success. Thus an alternate route was envisaged to obtain high quality nanocrystals of TiO₂ and ZnO with controlled size, morphology,

dispersability and without any coagulation using *in situ* surface modification through Hydrothermal, Solvothermal and Supercritical hydrothermal routes [2]. The size could be reduced significantly to a few nanometers without any coagulation and the organic coating was so much uniform and thin, that did not alter the inherent properties of metal oxide core. The organics which are insoluble and exist as separate phases under ordinary conditions became homogeneous phases under hydrothermal / solvothermal conditions. The small size and high surface to volume ratio of the individual nanoparticles imparts distinct size tunable physical and electronic properties that have prompted some to refer to them as “artificial atoms” [3]. A highly controlled self-assembly of these hybrid nanocrystals when dispersed in organic solvents into two-dimensional and/ or three-dimensional ordered structures or superlattice structures remains a relatively unexplored area. The mechanism of formation of organic-inorganic hybrid nanocrystals is very important. Here, theory of mechanism of the formation of organic-metal oxide interface has been discussed in detail with specific case studies. Another greatest advantage of such an *in situ* modification is that the nanocrystals surfaces could be made either hydrophobic or hydrophilic. The organics could be easily removed through sintering at around 500°C, such that crystals still remain as individual nanocrystals with controlled size and morphology. Experiments were carried out within the temperature range 150 – 250°C with autogeneous pressure. The run products were characterized using powder XRD, FTIR, UV-VIS, Positron annihilation lifetime and photoluminescence spectroscopy, TEM, SEM, etc. followed by a systematic evaluation of photocatalytic properties through degradation of toxic organic industrial effluents and waste. Thus the nanohybrid metal oxide crystals could be the most effective and prospective materials for environmental issues.

[1] A. Fujishima, K. Honda, *Nature* **1972**, *238*, 37-38. [2] T. Adschiri, K. Byrappa, In: *Nanohybridization of Organic-Inorganic Materials*, Eds: Atsushi Muramatsu, **2009**, Springer-Verlag, Germany. 217-250. [3] D.V. Shevchenko, D.V. Talapin, C.B. Murray, S. O'Brien, *J. Am. Chem. Soc.* **2006**, *128*, 3620-3637.

Keywords: metal oxide-organic hybrid nanocrystals, in situ surface modification, photocatalysis

MS49.P03

Acta Cryst. (2011) **A67**, C532-C533

Study of the intercalation of organic molecules into Hydrotalcite by fast in situ XRPD

Eleonora Conterosito,^a Marco Milanese,^a Luca Palin,^a Wouter Van Beek,^c Luana Perioli,^b Davide Viterbo,^a Gianluca Croce,^a ^a*Dipartimento di Scienze e Tecnologie Avanzate and Nano-SiSTeMI Interdisciplinary Centre, Università del Piemonte Orientale “A. Avogadro” (Italy)*. ^b*Dipartimento di Chimica e Tecnologia del Farmaco, Sezione di Tecnologie Farmaceutiche, Università di Perugia (Italy)*. ^c*Swiss-Norwegian Beamlines, ESRF, BP 220, F-38043 Grenoble Cedex, (France)*. E-mail: eleonora.conterosito@mfn.unipmn.it

A new mild and fast solid state [1] for the preparation of exchanged layered double hydroxide materials (LDH), in particular, for the intercalation of bioactive molecules was extended and adapted from the intercalation of phenylbenzimidazolsulfonic acid to two other kind of compounds. The chosen organic guest were 3-carboxy-coumarin and, given their importance, a series of non-steroidal-anti-inflammatory-drugs with different pka and steric hindrance; namely Ketoprofen, Flurbiprofen, Ibuprofen, and Tiaprofenic acid.

The mechanical mixture of the LDH-NO₃ and the guest compound was put in a capillary and then dampened with a drop of NaOH solution causing the intercalation to take place. The characterization of the