

MS10.08.03 ANOMALOUS SCATTERING POWDER DIFFRACTION: A VERSATILE TOOL. A. P. Wilkinson, School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA 30332-0400

Anomalous scattering diffraction facilitates two types of experiments, i) studies requiring scattering contrast variation, and ii) crystallographic site specific X-ray absorption measurements. In principle, the latter can provide information on local coordination geometry, oxidation state and polarization dependent effects for a specific crystallographic site, even when polycrystalline samples are used. The theory and experimental considerations involved in both types of experiments will be outlined and illustrated with examples of work on high T_c superconductors, zeolites, magnetic materials, and mixed valence compounds.

MS10.08.04 DISCUSSION ON EXPERIMENTAL TECHNIQUES FOR X-RAY COMPUTED DEPTH PROFILING. Kun Tao and Jian Luo, Dept. of Materials Sci. & Engr., Tsinghua Univ., Beijing 10084, P.R.China

The experimental techniques for X-ray Computed Depth Profiling (CDP) method [J. Luo, H. Yin & K. Tao, *Acta Physica Sinica* (Chinese Edition), 44.1788; J. Luo & K. Tao, *Acta Physica Sinica*, 44.1793, J. Luo & K. Tao, *Thin Solid Films*, in press] are discussed. X-ray polycrystalline diffraction data observed at various incident angles are used in determination of true phase-depth profiles for samples both with and without preferred orientation. Furthermore, numerical procedures are employed for solving the XRD patterns corresponding to every thin layer at arbitrary depth of a sample, which is similar to computed tomography technique. It has prospective application in determination of the true depth profiles of all structural information which can be obtained from X-ray peak intensity, peak position and line profile.

In the present paper, several selective topics were discussed in details. Determination of geometrical factor from a standard sample is discussed; different experimental methods and numerical procedures are compared; in addition, instrumentation and the scheme for samples with preferred orientation are also discussed.

MS10.08.05 MAGNETISM AND NEUTRON POWDER DIFFRACTION. F. Bourée, Laboratoire Léon Brillouin (CEA-CNRS), CEA/Saclay, F-91191 Gif-sur-Yvette, France.

Magnetic structure determination (description of the microscopic arrangement of magnetic moments in a crystal) requires neutron diffraction studies. Magnetic neutron powder diffraction is, and will remain in the future, the most straightforward technique to get magnetic structures as a function of temperature. We will show here the successive steps of a magnetic structure determination, from the experiment (2-axis diffractometer, sample environment) to the results: commensurate and/or incommensurate long-range magnetic order, via data analysis (Rietveld profile refinement). Some examples are selected, in RT_2X_2 , R_2T_2X and AB_2O_4 systems (with R= Lanthanide or Uranium; T, A, B=Transition Metal, X=Si, Ge, In or Sn).

MS10.08.06 EFFECT OF Ca SUBSTITUTION ON THE ROOM TEMPERATURE STRUCTURE OF $Sr_{1-x}Ca_xTiO_3$: A POWDER NEUTRON DIFFRACTION STUDY. Rajeev Ranjan and Dhananjai Pandey, School of Materials Science and Technology, Banaras Hindu University, Varanasi-221005, India.

Superlattice reflections observed for the first time in the room temperature powder neutron diffraction patterns of $(Sr_{1-x}Ca_x)TiO_3$, $x > 0.12$ are shown to arise due to an orthorhombic distortion of the perovskite structure. A Rietveld analysis of the neutron powder diffraction profiles shows that the structure consists of tilted TiO_6 octahedra and off-centred A-site cations. These novel structural features have important bearing on the quantum ferroelectric behavior of this system. Our work confirms the suggestion of Kleeman and Schremmer [*Phys. Rev. B* **40** (1989) 7428] that Ca induced electric dipoles responsible for quantum ferroelectricity in $(Sr,Ca)TiO_3$ results from off-centre occupancy of Ca along $\langle 110 \rangle$ of the perovskite unit cell. We show that the presence of tilted TiO_6 octahedra in the structure forces A-site cations to occupy off-centre positions for steric reasons. We do not find any evidence for the presence of Ca at the Ti site, postulated by Bednorz and Muller [*Phys. Rev. Lett.* **52** (1984) 2289], as the source of Ca induced electric dipoles. Neutron scattering was ideally suited for settling this issue since the neutron scattering lengths of Ca and Ti are of opposite sign.

MS10.08.07 CHARACTERIZATION OF MULTILAYERS AND THIN FILMS BY HIGH RESOLUTION X-RAY DIFFRACTION AND X-RAY STANDING WAVES Mikhail Kovalchuk, Svetlana Zheludeva, X-Ray Optics and Synchrotron Radiation Laboratory, A.V. Shubnikov Institute of Crystallography Russian Academy of Sciences, Leninsky pr.59, Moscow 117333, Russia.

X-Ray Standing Waves (XSW) method (see f.e. [1]) is based on the combination of high structural sensitivity of classical X-Ray diffraction method and spectroscopic selectivity under non-elastic secondary radiation measurements (photoelectrons, fluorescence, etc.). Surface-sensitivity of XSW is determined either by very small escape depth of secondary radiation and/or very small penetration depth for incident X-Ray under Total External Reflection conditions.

Present paper demonstrates unique possibilities of various modifications of XSW [2-4] for characterization of ultra-thin (crystalline and amorphous, inorganic and organic) layers, multi-layers systems and superlattices available due to the achievements of nanotechnology which allows to manipulate with ultra-thin layers constructing on their base absolutely new nanometer-scale materials (wave-guide structures and multilayers) and devices.

Different non-traditional ways in order to generate XSW (various kinds of secondary radiations and various types of interference phenomena) with period in the range: $0.1 \text{ \AA} - 1000 \text{ \AA}$ are discussed.

- [1] M.V. Kovalchuk, V.G. Kohn. *Sov. Phys. Usp.* **29**, (1986), 426.
- [2] M.V. Kovalchuk, A. Yu. Kazimirov, S.I. Zheludeva. *Nucl. Instrum. and Methods B* **101**, (1995), 435-452.
- [3] M.V. Kovalchuk, S.I. Zheludeva. *Journal de Physique IV, Colloque C9, Suppl. au Journal de Physique III, Vol.4, November 1994*, C9-431.
- [4] S.I. Zheludeva, M.V. Kovalchuk, N.N. Novikova, A.N. Sosfenov. *Advances in X-Ray chemical analysis*, **26S**(1995), 181.