

Poster Sessions

Chem. **2010**, 6223-6225; T.C. Harrop, Z.J. Tonzetich, E. Reisner, S.J. Lippard *J. Am. Chem. Soc.* **2008**, 130, 15602-15610; Z.J. Tonzetich, H.L. Do, S.J. Lippard *J. Am. Chem. Soc.* **2009**, 131, 7964-7965.

Keywords: cluster, iron, spectroscopy

MS56.P14

Acta Cryst. (2011) **A67**, C587

Effects in the atomic structure of BaFe₂As₂ by pressure and chemical substitution

E. M. Bittar,^a E. Granado,^{b,a} L. Mendonça-Ferreira,^c F. Garcia,^a G. de M. Azevedo,^d C. Adriano,^b T. M. Garitezi,^b L. F. Bufaiçal,^c P. G. Pagliuso,^b ^aLaboratório Nacional de Luz Síncrotron, Campinas, SP, (Brazil). ^bInstituto de Física "Gleb Wataghin", UNICAMP, Campinas, SP, (Brazil). ^cInstituto de Física e Matemática, UFPel, Pelotas, RS, (Brazil). ^dInstituto de Física, UFRGS, Porto Alegre, RS, (Brazil). ^eInstituto de Física, UFG, Goiânia, GO, (Brazil). E-mail: eduardo.bittar@lnls.br

The effects of K and Co substitutions and quasi-hydrostatic applied pressure ($P < 9$ GPa) in the local atomic structure of BaFe₂As₂, Ba(Fe_{0.937}Co_{0.063})₂As₂ and Ba_{0.85}K_{0.15}Fe₂As₂ superconductors were investigated by extended X-ray absorption fine structure (EXAFS) measurements in the As *K* absorption edge. The As-Fe bond length is found to be slightly reduced (d 0.01 Å) by both Co and K substitutions, without any observable increment in the corresponding Debye-Waller factor. Also, this bond is shown to be compressible ($\kappa = 3.3(3) \% 10^{-3}$ GPa⁻¹). The observed contractions of As-Fe bond under pressure and chemical substitutions are likely related with a reduction of the local Fe magnetic moments, and should be an important tuning parameter in the phase diagrams of the Fe-based superconductors.

Keywords: pnictides, superconductivity, EXAFS

MS56.P15

Acta Cryst. (2011) **A67**, C587

Anisotropy in Anomalous Scattering in TiO₂ and the influence of point defects

Carsten Richter,^{a,b} Matthias Zschornak,^a Dmitri Novikov,^b and Dirk C. Meyer,^a ^aInstitute of Experimental Physics, TU Bergakademie Freiberg, (Germany). ^bHamburger Synchrotronstrahlungslabor HASYLAB at DESY, (Germany). E-mail: carsten.richter@desy.de

Diffraction intensities near an absorption edge of one of the crystal's atoms show a considerable dependency on the polarization of the incident and scattered X-rays and also on the corresponding wave vectors called Anisotropy in Anomalous Scattering (AAS). The polarization is usually varied by rotating the crystal around the momentum transfer vector by an angle ψ . Based on the tensorial treatment of this dependency like described by Kirfel et. al. [1], we studied the forbidden reflection 001 and the allowed reflection 111 of rutile at the titanium K absorption edge. Furthermore we investigated the influence of diluted point defects, in particular oxygen vacancies, on the scattered intensity profiles. Point defects as one possible origin for polarization anisotropy were discussed by Dmitrienko et. al. [2] which formed the basis of our considerations. Variations of the AAS profiles with energy have been observed and theoretically been account for. For the allowed 111 reflection a clear change of these patterns with increasing number of oxygen vacancies has been measured at different beamlines of the light source DORIS at DESY.

[1] A. Kirfel, A. Petcov, K. Eichhorn, *Acta Cryst.* **1991**, *A47*, 180. [2] V.E. Dmitrienko, E.N. Ovchinnikova: *Acta Cryst.* **2000**, *A56*, 340.

Keywords: DAFS, rutile, AAS

MS56.P16

Acta Cryst. (2011) **A67**, C587

The Structure and X-ray Absorption Spectrum Studies of Mn and N Co-doped ZnO

H. H. Hsieh,^a N. Niu,^b C. H. Chen,^b M. D. Lan,^c H. F. Huang,^c ^aCheng Chung Institute of Technology, National Defense University, (Taiwan), R.O.C., ^bNuclear Science and Technology Development Center, National Tsing Hua University, Hsinchu, (Taiwan), R.O.C. ^cDepartment of Physics, National Chung Hsing University, Taichung, (Taiwan), R.O.C. E-mail: hhsieh@ndu.edu.tw

To grow ferromagnetic *P*-type Zn(Mn)O, nitrogen and manganese co-doped ZnO film with wurtzite structure were made by ion implantation method. The Mn *K*-edge and *L*_{3,2}-edge peaks of samples have same binding energy with peak of MnO. So the X-ray absorption spectrum show the valence of doped Mn ion is 2+. The ions substitution of Zn by Mn was proved. The X-ray diffraction show a extra peak about 1.3 degree lower than the ZnO(200) peak at 66.39 degree. The lattice length became longer after doping. The Curie temperature, coercive, and saturation moment were measured by SQUID. All of them were tuned by the controlling of nitrogen concentration. The effective magnetic moment and pinning force were enhanced but the Curie temperature was decrease upon the doped nitrogen concentration. The nitrogen substitution for oxygen can change not only carrier concentration but also the magnetic coupling strength between neighboring Mn ions.

Keywords: ZnO, X-ray absorption spectrum

MS56.P17

Acta Cryst. (2011) **A67**, C587-C588

XRD and dual elemental XAFS analyses of inorganic solids

M. E. Montero-Cabrera,^a L.E. Fuentes-Cobas,^a E. Macías-Ríos,^a J. Soto-Nuñez,^b M. García-Guaderrama,^c M. E. Fuentes-Montero,^d E. Morán,^c M.A. Alario-Franco,^c ^aCentro de Investigación en Materiales Avanzados, Chihuahua, Chih., (Mexico). ^bFacultad de Ingeniería, Universidad Autónoma de Chihuahua, Chihuahua, Chih., (Mexico). ^cDepartamento de Ingeniería de Proyectos, Universidad de Guadalajara, Zapopan, Jal., (Mexico). ^dFacultad de Ciencias Químicas, Universidad Autónoma de Chihuahua, Chihuahua, Chih., (Mexico). ^eDepartamento de Química Inorgánica, Facultad de Ciencias Químicas, Universidad Complutense de Madrid, Madrid, (Spain). E-mail: elena.montero@cimav.edu.mx

Two inorganic solid solutions, γ -Fe_{2-x}Cr_xO₃ and LaFeNiTiO₃, were studied by X-ray absorption fine structure (XAFS) of K-absorption edge of two elements and by synchrotron radiation X-ray diffraction (XRD). Measurements were performed at the Stanford Synchrotron Radiation Lightsource at room temperature.

High-resolution XRD patterns were processed by means of the Rietveld method, using Fullprof [1]. In Rietveld refinements, the ordered/disordered degree of the considered solutions is indiscernible in cases of atoms being neighbors in the Periodic Table. Crystallographic interpretation of magnetic and ferroelectric phenomena is shortened by this limitation.

Double-element XAFS analysis was applied to clarify, via short-range structure characterization, the nature of investigated systems. In