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Keywords: cluster, iron, spectroscopy

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Effects in the atomic structure of $BaFe_2As_2$ by pressure and chemical substitution

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The effects of K and Co substitutions and quasi-hydrostatic applied pressure ($P < 9$ GPa) in the local atomic structure of $BaFe_2As_2$, $Ba(Fe_{0.937}Co_{0.063})_2As_2$ and $Ba_{0.85}K_{0.15}Fe_2As_2$ supercon-ductors 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

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

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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.

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Keywords: DAFS, rutile, AAS

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

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To grow ferromagnetic *P*-type Zn(Mn)O, nitrogen and mnganese 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

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XRD and dual elemental XAFS analyses of inorganic solids

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Two inorganic solid solutions, γ-$Fe_{2-x}Cr_xO_3$ and $LaFeNiTiO_3$, 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