

(Grenoble) ($\lambda=0.3748$ Å) at 25° and 250°C, respectively, suggests that the coefficient of thermal expansion is highest for samples with low iron substitution. Split of triangular Cu2 positions increases with temperature and the half-occupied Cu2 positions from different coordination triangles approach one another, down to 2.70-2.75 Å in tennantite at 250°C. There is insignificant residual electron density between the split Cu2 half-sites in tetrahedrite at 25°C and its increase with temperature is moderate. The inter-site density is substantially higher in tennantite and it increases considerably with temperature, especially in the low-Fe sample.

MS17 P23

Ion exchange properties for lamellar oxides

Nadia Belmokhtar, Ratiba Nedjar, Houria Rebbah

Laboratoire de Science des Matériaux 1, USTHB, BP32, El-Alia, 16111 Bab-Ezzouar, Alger, Algérie.

E-mail: Ratibanedjar@yahoo.fr

Keywords : partial exchange, soft chemistry, oxide

The investigations about materials dealing with energy have shown that the oxides with a layer structure are potential candidates for solid state electrolytes and for electrodes. In this respect, attention has been focussed on protonic oxides owing to their stability at rather high temperature. Moreover these latter compounds are characterized by their ability to accommodate in the interlayer space ions of different shapes and sizes. They offer the possibility to synthesize some partially exchanged compounds. During this work reactions of some K⁺ and Na⁺ salts (1) with the layered niobic acid HNb3O8 (2) in different ratio (1)/(2) were studied. The partial exchange reaction increases the spacing between the inorganic sheets is discussed in terms of ion size and state of hydration.

MS17 P24

Temperature dependent stability field of nanodomain structures in PZT ceramics using synchrotron powder diffraction Kristin A. Schoenau^a, Michael Knapp^b, Hans Kungl^c, Michael J. Hoffmann^c, Mario Maglione^d, Hartmut Fuess^a ^aMaterials Science, Darmstadt University of Technology, Germany. ^bCELLS, Barcelona, Spain. ^cInstitute of Ceramics in Mechanical Engineering, University of Karlsruhe, Germany ^dICMCB-CNRS, Université Bordeaux I, France.

E-mail: schoenau@matgeo.tu-darmstadt.de

Keywords: ferroelectric oxides, in situ synchrotron x-ray powder diffraction, phase stability, nanodomains,

Extraordinarily high piezoelectric properties of ferroelectric lead zirconate titanate, PbZr_{1-x}Ti_xO₃ (PZT), at its so-called morphotropic phase boundary (MPB) between tetragonal and rhombohedral symmetry have raised interest on the structural properties of this compositional area in last years. Discussions involved a coexistence of tetragonal and rhombohedral structures as well as the existence of a monoclinic phase [1]. Recent studies using high-resolution synchrotron x-ray powder diffraction in combination with TEM and EPR at ambient temperature [2, 3] were able to correlate XRD observation with a nanodomain structure. The internal symmetry of the nanodomains is difficult to determine due to strong coherence effects in diffraction experiments, which is in

correspondence with findings for relaxor ceramics using martensitic theory [4]. The fraction of nanodomains within the material besides tetragonal microdomains can be derived using a two-phase Rietveld fit. To investigate the stability field of these nanodomains with changes in temperature dependent on sample composition, in situ diffraction experiments on powders were conducted in transmission mode at the beamline B2, Hasylab, Hamburg Germany. Various parameters derived from Rietveld refinement are found to reflect the changes in domain structure. There are e.g. pronounced changes in volume strain of the tetragonal phase accompanied by the observation of a plateau in the evolution of the c/a-ratio of the tetragonal phase, as seen in Fig.1, which classify the stability range of the nanodomains.

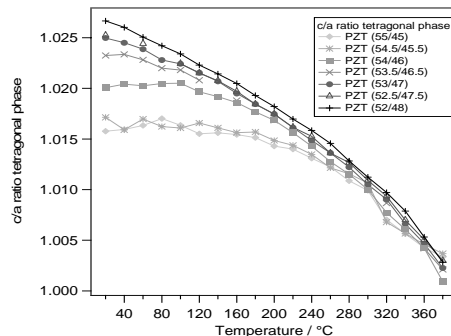


Fig. 1: Temperature-dependent evolution of the tetragonal c/a-ratio for samples out of the compositional range of the MPB.

- [1] Glazer, A. M.; Thomas, P.A.; Baba-Kishi, K. Z.; Pang, G. K. H.; Tai, C. W.; *Phys. Rev. B* 70, 184123 (2004)
- [2] Schmitt, L.A., Schönau, K.A.; Theissmann, R.; Fuess, H.; Kungl, H.; Hoffmann, M.J.; *J. Appl. Phys.* 101, 074107 (2007).
- [3] Schönau, K.A.; Schmitt, L.A.; Knapp, M.; Fuess, H.; Eichel, R.-A.; Kungl, H.; Hoffmann, M.J. *Phys Rev B*, 2007, 75(14) in press.
- [4] Jin, Y.M.; Wang, Y.U.; Khachatryan, A.G.; Li, J.F.; Viehland, D.; *J. Appl. Phys.*, 2003, 94 (5), 3629

MS17 P25

Peculiarity of polymerization of the fullerite C₆₀ in a hexagonal form. N.R. Serebryanaya^a, G.A. Dubitsky^a, V.D. Blank^a, B.N. Mavrin^b, E.A. Skryleva^c, E.V. Skokan^d, V.V. Aksenkov^a, ^aTISNCM, Troitsk, Russia, ^bInstitute of Spectroscopy, Troitsk, Russia, ^cMoscow Institute of Steel and Alloys, Russia, Department of Chemistry, MSU, Russia. E-mail: nadya@ntcstm.troitsk.ru

Keywords: fullerenes, polymerization, high pressure

2D polymerized phases of the hexagonal closed-packed (hcp) modifications of fullerite C₆₀ have been manufactured after the high-pressure-high-temperature treatment at 4 GPa and different temperatures. Polymeric phases of the hcp-form are compared with the polymeric phases of fcc-form obtained at the same conditions. Polymeric phases of both C₆₀ forms have been investigated by X-ray diffraction, X-ray photoelectron (XPS) and Raman spectroscopy methods. At 450° C the hcp-form is transformed into 2D polymeric rhombohedral phase as the fcc-form. The Raman spectra confirmed that 2D polymeric structures of C_{60_hcp} (orthorhombic and rhombohedral structures) are the same as these of C_{60_fcc}. Unit-cell parameters of 2D polymeric structures of C_{60_hcp} and C_{60_fcc} are calculated.