Keywords: electro-conductivity, thermoelectromotive, impurities

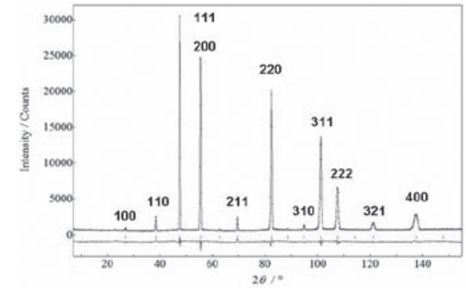
P11.13.84

Acta Cryst. (2008). A**64**, C533

Structural investigation of the cubic perovskite-type doped lanthanum cobaltite $La_{0.4}Ba_{0.6}CoO_{3-x}$

Takashi Ohta, Masatomo Yashima, Takahiro Wakita
Tokyo Institute of Technology, Department of Materials Science and Engineering, Interdisciplinary Graduate School of Science and Engineering, Nagatsuta-cho 4259-J2-61, Midori, Yokohama, Kanagawa, 226-8502, Japan, E-mail：ohta.takashi@ath.kuramae.ne.jp

Lanthanum strontium cobaltites, $La_{0.4}Ba_{0.6}CoO_{3-x}$, which have a perovskite-type structure, are promising electrode materials for solid oxide fuel cells (SOFCs). The purpose of the present study is to investigate the crystal structure of the cubic Pm-3m perovskite-type $La_{0.4}Ba_{0.6}CoO_{3-x}$ at room temperature and at high temperature by neutron diffractometry. Neutron diffraction data were collected in air by a diffractometer HERMES with a 150 multi-detector system. A furnace with $MoSi_2$ heaters was placed on the sample table, and used for neutron diffraction measurements at high temperatures (J. Am. Ceram. Soc. 85 (2002) 2925). The experimental data were analyzed assuming the cubic perovskite-type structure by Rietveld method. La and Ba atoms were placed at the special position 1b 1/2, 1/2, 1/2 of the Pm-3m symmetry. Co and O atoms were put at the 1a 0, 0, 0 and 3d 1/2, 0, 0 sites, respectively. The calculated profile agreed well with the observed one taken at room temperature (Figure). The refined crystal structure of $La_{0.4}Ba_{0.6}CoO_{3-x}$ is similar with that of cubic $La_{0.6}Sr_{0.4}CoO_{3-x}$ at 1531K reported in our previous work [J. Appl. Crystallogr., 40 (2007) 1166].



Keywords: neutron diffraction, solid oxide fuel cells, perovskite-type structure

P11.13.85

Acta Cryst. (2008). A**64**, C533

Synchrotron XRD and EXAFS studies on nanocrystalline ZrO_2-CaO solid solutions

Ismael O Fabregas[1], Diego G Lamas[1], Walsoe de Reca E Noemi[1], Marcia C.A Fantini[2], Aldo F Craievich[2], Rogerio J Prado[3]
[1]CITEFA, CINSO, JB de Lasalle 4397, Villa martelli, Buenos Aires, B1603ALO, Argentina, [2]Universidade de Sao Paulo, Travessa R da Rua do Matao, no.187, Cidade Universitaria, 05508-900, Sao Paulo, Brazil, [3]Universidade Federal de Mato Grosso, Av. Fernando Correa s/n, 78060-900, Cuiaba - MT, Brazil, E-mail：ifabregas@citefa.gov.ar

The crystal structure and the local atomic order of a series of nanocrystalline ZrO_2-CaO solid solutions with varying CaO content were studied by synchrotron radiation X-ray powder diffraction and extended X-ray absorption fine structure (EXAFS) spectroscopy. These samples were synthesized by a pH-controlled nitrate-glycine gel-combustion process. For CaO contents up to 8 mol%, the t ´ -form of the tetragonal phase ($c/a > 1$) was identified, whereas, for 10 and 12 mol% CaO, the t“-form ($c/a = 1$; oxygen anions displaced from their ideal positions in the cubic phase) was detected. Finally, the cubic phase was observed for solid solutions with CaO content of 14 mol% CaO or higher. Thus, the t ´ /t“ and t“/cubic compositional boundaries were determined to be at (9 ± 1) and (13 ± 1) mol% CaO, respectively. EXAFS study demonstrated that this transition is related to a tetragonal-to-cubic symmetry change of the first oxygen coordination shell around Zr atoms.

Keywords: zirconia, XAFS, synchrotron X-ray diffraction

P11.13.87

Acta Cryst. (2008). A**64**, C533

Novel long period structures in hydrogen storage $La_xY_{1-x}Ni_{3.8}$ compounds

Ryo Ishikawa[1], Eiji Abe[1], Kazuhiro Ishikawa[2], Kiyoshi Aoki[2]
[1]The university of Tokyo, Materials engineering, 7-3-1 Hongo, Bunkyo-ku, Tokyo, 81, Japan, [2]Kitami Institute of Technology, 165 Koen-cho, Kitami, Hokkaido, 81, Japan, E-mail：ishikawa@stem.t.u-tokyo.ac.jp

A series of (La,Y)Niz ($3< z <4$) alloy compounds show polymorphic block-stacking superstructures. These structures can be interpreted as rombohedral stacking sequence of ABC (3R-type) and hexagonal stacking sequence of AB (2H-type), where the structural unit is composed of $LaNi_5$ (Haücke phase) and YNi_2 (Laves phase, C15) type structures at unit-cell scale. In this presentation, we describe the differences of local chemistry between non-reacted and after gaseous-H2 reacted (La,Y)Niz ($3< z <4$) compounds through the direct observation by Z-contrast scanning transmission electron microscopy (STEM). All of $(La_x,Y_{1-x})Ni_{3.8}$ (x=0.4,0.5,0.6) superstructures annealed at 1023K for 14 days are identified as 5:19R-type (3R) [1] based on electron diffraction analysis. Interestingly, for all the images there appear Z-contrast modulations at nanometer scales, which become significant for the $La_{0.6}Y_{0.4}Ni_{3.8}$. These directly represent local chemical fluctuations, namely the occurrence of La-rich/Y-rich chemical domains in these alloys: that is to say, ‘chemical mosaicness’. STEM image of $La_{0.6}Y_{0.4}Ni_{3.8}$ reacted with 2MPa hydrogen shows disappearance of ‘chemical mosaicness’, and to transform a novel long period Y-ordered 9R superstructure with c-length approximately 167Å. On the basis of Z-contrast analysis, we find that the novel structure contains Y-hydride layers, whose structure is well interpreted by referring structure local atomic configurations within YH_3 compound.

References

[1] T. Ozaki, et al., J. Alloys Compd., 446-447, (2007) 620-624.

Keywords: hydride compounds, STEM, chemical domain structure

P11.13.88

Acta Cryst. (2008). A**64**, C533−534

Structural investigation of the Ba doped $LaInO_3$

Park HyunMin[1], Chung Sujin[2]
[1]Korea Research Institute of Standards and Science, Div. of Advanced Technology, 1 Doryong-Dong,, Daejon, Yuseong-Gu, 305-600, Korea (S), [2]School of Materials Science and Engineering, Seoul National University, Seoul 151-742, Korea, E-mail：hmpark@kriss.re.kr

A high ionic conductor Ba doped lanthanum indium oxide was investigated by synchrotron powder diffraction and transmission