Poster Sessions

Voltage Electron Microscope). EF-PED data resulted in the basic crystallographic information of ZnS nano-crystals: P63mc, a = 3.83Å and c = 6.26Å; F-43m, a = 5.41Å, respectively. As a result of HREM analysis, their crystallite shapes were turned out to be nano-rods and nano particles, respectively and the nano-rod structure was elongated to the [001] direction. The size and shape dependency related to crystal structures of ZnS nano-crystals has been discussed.



Fig. 1. EF-PED and HREM analysis of ZnS nano-crystals. (a) Cubic structure of ZnS nano particles. (b) Hexagonal structure of ZnS nano-rods

Keywords: electron crystallography, energy-filtered precession electron diffraction, ZnS

P19.03.09

Acta Cryst. (2008). A64, C605

Electrostatic potential analysis of the orbital-ordered phase of spinel oxide FeCr₂O₄ using CBED

Daisuke Morikawa, Kenji Tsuda, Shintaro Ohtani, Takahisa Arima Tohoku University, Institute of Multidisciplinary Reserch for Advanced Materials, 2-1-1 Katahira, Aoba-ku, Sendai, Miyagi, 980-8577, Japan, E-mail:morikawa@mail.tagen.tohoku.ac.jp

A structure analysis method using convergent-beam electron diffraction (CBED), which was developed by Tsuda and Tanaka[1,2], enables us to directly determine the electrostatic potential from a nanometer-scale specimen area. The electron density distribution can be also obtained from the electrostatic potential through the Poisson's equation. We have applied the method to a spinel oxide FeCr₂O₄, which undergoes a structural phase transformation at 135K from a cubic spinel structure of the high-temperature phase to a tetragonal structure of the low-temperature phase with Jahn-Teller(JT) distortion[3]. A ferro-type orbital-ordering of 3d electrons of Fe atoms is expected in the low-temperature JT-distorted phase of FeCr₂O₄[4]. FeCr₂O₄ single crystals were grown by the chemical vapor transport(CVT) method. Energy-filtered CBED patterns of the low-temperature phase were obtained at a specimens temperature of 90K using an energy-filter transmission electron microscope(EFTEM) JEM-2010FEF with an accelerating voltage of 100kV. Atom positions, Debye-Waller factors and low-order structure factors were refined by nonlinear least squares fitting between the experimental CBED patterns and dynamical diffraction calculations using an analysis software MBFIT[1]. The electrostatic potential and electron density distributions were reconstructed from the refined parameters. Clear anisotropy of the electrostatic potential has been found, which is attributed to the ferro-type ordering of the $3z^2-r^2$ orbitals of the Fe atoms.

References:[1]K. Tsuda & M. Tanaka, *Acta Cryst.* A**55**, 939-954(1999). [2]K. Tsuda et al., *Acta Cryst.* A**58**, 514-525(2002). [3]G.Shirane. *J. Appl. Phys.* **35**, 3(1964). [4]T.Arima et al., *J. Magn. Magn. Mat.* **310**, 807(2007).

Keywords: CBED, electrostatic potential, spinel

P19.03.10

Acta Cryst. (2008). A64, C605

Microstructural characterization of YPO₄: Li by transmission electron microscopy

Lucia Diaz-Barriga¹, Ivonne Rosales², Lauro Bucio²

¹ESIQIE/ Instituto Politecnico Nacional, Metralurgia, Av.IPN S/N colonia Lindavista, MEXICO DF, DF, 07300, Mexico, ²Instituto de Fisica, Universidad Nacional Autonoma de Mexico, Apdo. Postal 20-364, 01000 Mexico DF, Mexico, E-mail:luchell@yahoo.com

Xenotime YPO ₄ is an yttrium phosphate with a tetragonal structure and can be doped by ions of diverse diameters in order to control its electrical conductivity. The purpose of this work is to present an study about the microstructural characterization of YPO ₄ by electron transmission microscopy when this yttrium phosphate is doped with lithium. Samples were obtained by the following solid state reaction: $Y_2O_3 + (NH_4)_2HPO_{4^{--}} > YPO_4$:xLi Powder samples were studied in a JEOL 100 CX with point resolution of 2.7angstrom . Bright field and Diffraction techniques were used to establish that YPO ₄:xLi has an orthorhombic structure with lattice parameters: a=b=9.7 angstrom and c= 6.01 angstrom ,this means that intersticial lithium ions can create a distortion in the tetragonal structure of yttrium phosphate.

Keywords: xenotime, orthorhombic yttrium phosphate, electron microscopy

P19.04.11

Acta Cryst. (2008). A64, C605-606

Determination of chiral indices of carbon nanotubes using electron diffraction pattern

<u>Yohei Sato¹</u>, Kenji Tsuda¹, Masami Terauchi¹, Yahachi Saito² ¹Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai, Miyagi, 980-8577, Japan, ²Department of Quantum Engineering, Nagoya University, Furou-chou, Chikusa-ku, Nagoya 464-8603, Japan, E-mail:y-sato@tagen.tohoku.ac.jp

Carbon nanotubes (CNTs) show physical properties of a metal or a semiconductor depending on these structures. Thus, it is important to investigate the structure of a single CNT expressed by a chiral index (n, m) [1]. Transmission electron microscopy is a powerful tool to investigate structures of single CNTs. In the present study, the chiral indices are determined by using electron diffraction patterns obtained from single double-walled CNTs (DWCNTs) and single single-walled CNTs (SWCNTs). Electron diffraction patterns were obtained from 200 nm areas containing a single DWCNT or SWCNT by using a transmission electron microscope of JEM2010 at an accelerating voltage of 100 kV. Intensities of the diffraction patterns were recorded on imaging plates. Determination process of chiral indices is as follow. 1. The chiral angles and diameters of the CNT are estimated from the diffraction patterns. 2. The chiral indices (n, m) of the CNT are estimated from the angles and the diameters. 3.Diffraction patterns of chiral indices (n, m) were simulated using a simulation program "MBFIT" [2, 3]. 4. The simulated diffraction patterns are compared with the experimental patterns. 5. Chiral indices (n, m) were determined from the best agreement between the experimental and the simulated patterns. The determination of chiral indices enables us to calculate the joint densities of states of the CNTs and to compare electron energy-loss spectra of the CNTs with joint density of states of the CNTs calculated from chiral indices (n, m).