

FA5-MS06-P07

Pressure Induced Phase Transformations in the Partially Filled Clathrate $\text{Rb}_{6.15}\text{Si}_{46}$. Denis Machon^c, Pierre Toulemonde^b, Paul F McMillan^e, Mónica Amboage-Castro^a, Alfonso Muñoz^d, Plácida Rodríguez-Fernández^d, Alfonso San-Miguel^c.

^aEuropean Synchrotron Radiation Facility, Grenoble, France. ^bInstitut Néel, CNRS and Université Joseph Fourier, Grenoble, France. ^cLPMCN, Université Lyon-I and CNRS, France. ^dUniversidad de La Laguna, La Laguna, Tenerife, Spain. ^eUniversity College London, London, UK.

E-mail: sanmiguel@lpmcn.univ-lyon1.fr

Group 14 clathrates constitute prototype systems for the study of host-guest interactions at the nanoscale [1]. Type-I clathrates are made of the crystalline assemblage of silicon nanocages of 24 and 20 atoms having the possibility for the endohedral inclusion of guest atoms. The high pressure evolution of group 14 clathrates include a number of intriguing phase transitions including an homothetic isostructural volume collapse or a pressure induced amorphisation [2]. One method to better understand the importance of host-guest interaction in their pressure evolution is to consider the study at partial nanocage filling. The type I clathrate $\text{Rb}_{6.15}\text{Si}_{46}$ with partly empty cages has been studied up to 36 GPa using Raman spectroscopy, synchrotron x-ray diffraction in diamond anvil cells, and ab initio total-energy and lattice-dynamics calculations. A first phase transition is observed at 13 ± 1 GPa, and a “volume collapse” transition within the clathrate structure is then observed at 24 ± 1 GPa. Pressure-induced amorphisation into a high-density amorphous (HDA) state occurs above $P = 33 \pm 1$ GPa. The HDA form transforms into a low-density amorphous polymorph (LDA) during decompression. During the compression study using angle dispersive synchrotron x-ray diffraction techniques we measured bulk modulus parameters for rocksalt-structured TaO for the first time, included adventitiously in the clathrate sample ($K_0 = 293(3)$ GPa and $K'_0 = 5.4(3)$).

[1] A. San Miguel, *Chemical Society Reviews*, 35, 876-889, 2006.

[2] A. San Miguel and P. Toulemonde, *High Pressure Research*, 25, 159, 2005.

Keywords: high pressure; clathrates

FA5-MS06-P08

Microstructure of Yb Substituted Y_2O_3 from HRTEM and X-ray Diffraction Approaches. Bratislav Antic^a, Aleksandar Kremenovic^a, Milica Vucinic-Vasic^a, Aleksandar S. Nikolic^b. ^aThe “Vinca” Institute, Belgrade, Serbia. ^bFaculty of Chemistry, University of Belgrade, Belgrade, Serbia.

E-mail: bantic@vinca.rs

The mixed sesquioxides, $\text{Y}_{2-x}\text{Yb}_x\text{O}_3$ ($x=0.06, 0.10, 0.20, 0.40$) with particles of 5 nm were studied by HRTEM and X-ray diffraction technique approaches. Rietveld refinement

of occupation numbers shows a preferential Yb^{3+} toward to C_3 sites in the Ia3 space group for concentration $x \leq 0.20$, and become random for $x=0.40$. From optical point of view, site distribution of active centers in host matrices is important. The sample with $x=0.20$, where a random distribution of Yb^{3+} was found, is most suitable sample for optical applications. Electron transmission microscopy is used in order to obtain information about sizes, size distribution, defects and morphology of nanoparticles. Distribution of the particles is narrow and most of particles are approximately 5 nm in diameter. The particles are homogeneous, without visible shell in particle or amorphous phase in sample. At nanoscale, particles can be described by core/shell model. The particles are probably without shell, or with very tiny shell which are not detected by the used experimental techniques. Crystallite size distribution obtained from Breadth computer program is compared from one determined by HRTEM. Although, both of them show the similar values for the large number of particles/crystallites, there is a discrepancy between two distribution for small particles/crystallite values. The disagreement is based on the basic principles of methods and mathematical models that were used. Crystallite size determined by X-ray diffraction technique is close to particle size determined from HRTEM, indicating that particles are composed from one crystallite in average. X-ray line broadening analysis show negligible anisotropy of X-ray line broadening provoked by the strain and size effects.

In conclusion, we develop a method for production of rare earth oxides based nanophosphors using thermal decomposition of acetylacetonato (AcAC) complexes and it was applied here for formation of monodispers nanoparticles. Crystallographic study show that the method could be used in commercial production of rare earth based nanophosphors.

Keywords: microstructures; nanoparticles; oxides

FA5-MS06-P09

Effect of Sign Reversal by Misorientation Vector along Block Boundaries and its Detection.

Vyacheslav Malkov^a, Victor Strekalovsky^a, Andrey Malkov^b, Oleg Malkov^b, Vladimir Puchin^c. ^aInstitute of High-Temperature Electrochemistry, Ural Branch RAS. ^b“ROSNA” Scientific and Production Center. ^cInstitute of Metal Physics, Ural Branch RAS, Ekaterinburg, Russia.

E-mail: mvb@ihte.uran.ru

Studies performed in the field of nanotechnologies necessitate exploration and testing of nanomaterials. Similarly to microscale materials, nanomaterials can be in the elastodeformed state [1]. Such nanomaterials include flat nanothin diamond-shaped crystals of hexagonal selenium growing in amorphous films at crystallization temperatures of $180 \div 160^\circ\text{C}$. The lattice of these crystals has a nonuniform rotational distortion about the C-axis whose direction coincides with the short diagonal of the diamond-shaped crystal. Relaxation of the elastodeformed state in some area of the diamond-shaped nanothin crystal results