and low (~10^9 cm^{-2}) dislocation density has been characterized as cell walls and cell interiors respectively with compressive and tensile stresses in accordance with the quasi-composite model. The results are in gross agreement with earlier TEM studies.

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Keywords: composites, X-ray diffraction, dislocation structure

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Strain-free Oxide Nanopowders, Facts and ex-Oxalate MgO Case

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The microstructural characterization of nanocrystalline materials is of particular importance in the study of chemical fragmentation processes and oxides prepared from solution routes. Only a few examples of strain-free (i.e. with negligible microdistortion) oxides have been reported. Their preparation is often not trivial, since the chemical nature of the precursor used and the experimental conditions can influence the microstructural properties. Representative examples of strain-free oxides are ZnO [1], CeO_2 [2] and Y_2O_3 [3]. A new example, i.e. nanocrystalline MgO obtained from the thermal decomposition of the oxalate precursor is investigated in detail. The study is based on line broadening analysis carried out with the Voigt/Langford integral breadth and Fourier methods combined with the pattern decomposition technique. The whole pattern refinement method is also applied. A good agreement between the results obtained from the varied approaches is found. Ex-oxalate MgO is strain free. The crystallites are, on average, isotropic with sizes increasing from 130 Å to 640 Å in the annealing temperature range 500-1200°C and crystallite growth varies exponentially. The results obtained from the different methods are discussed and are also compared to those observed with MEB and BET techniques.

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Keywords: line profile analysis, microstructure, nanoparticles

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Geterostructures of Bacterial Cellulose Acetobacter Xylinum Intercalated by Drug Materials

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Organic-inorganic hybrid materials based on bacterial cellulose with metal nanoparticles are interesting for medical applications. High-crystal cellulose matrix obtained at static growth of Acetobacter Xylinum (AX) in the process of intercalation of drugs was investigated by methods of small and wide-angle X-ray scattering, electron diffraction, transmission electron microscopy and atomic force microscopy.

The investigation of interaction of polyvinilpyrrolydone (PVP) and germicide preparation Poviargol and Catapol (Ag° and Se° nanoparticles stabilized by PVP) with gel-films AX by diffraction methods has shown that besides reflections associated with crystal-state cellulose, in both cases reflections from PVP phase are present. In the case of gel-films AX with Poviargol the reflections are observed from silver. Small-angle X-ray scattering experiments with composite samples allowed us to estimate the relative amount of intercalated PVP, Ag and Se in the process of their desorption by substituion with water, and to determine the size distributions of the nanoparticles. The distributions show relatively large amount of small particles (5-20nm) and minority of larger ones (up to 100nm).

Keywords: electron and X-ray diffraction, bacterial cellulose, organic-inorganic hybrid materials

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Honeycomb Diffuse Intensities in $NaREF_4$ Upconversion Materials

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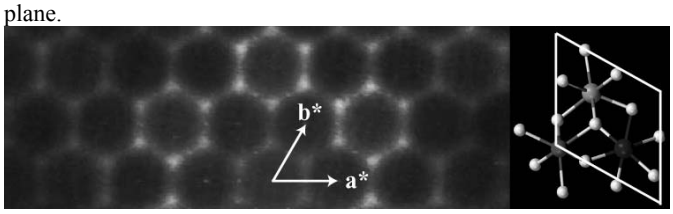
Hexagonal sodium rare-earth (RE) fluorides, e.g. NaYF4: Yb, Er, are very efficient upconversion materials which emit visible light upon infrared excitation. The efficiency of the upconversion process depends mainly on the doping ratio, the phase purity and the Na:RE ratio. These phases have hexagonal structures with a disordered cation distribution. Here we report a detailed investigation of $Na_{1.5}La_{1.5}F_6$. The reconstructed layers of reciprocal space contain either sharp Bragg reflections for integer values of *l*, or planes with honeycomb like diffuse intensities for half-integer values of *l* (Fig left: *h k* 1.5). The Bragg reflections indicate a hexagonal metric and the average structure could be refined with space group symmetry *P*-6. It shows three different columns of cations with Na, La or a 1:1 ratio of both (Fig right). The diffuse intensities are well reproduced if it is assumed that Na and La alternate regularly in the disordered columns along **c** and that Na and La alternate with a probability less than one in the **a**,**b** plane.



Keywords: disordered materials, diffuse scattering, phosphors

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Stacking Faults and Internal Strains in DHCP Phase of La

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High-resolution synchrotron X-ray diffraction measurements of La have been carried out in the range of temperatures from 80 K to 800 K at ambient pressure. The powder diffraction patterns contained characteristic features of DHCP crystals with stacking faults. Additional peak broadening was attributed to a lattice strain. A considerable amount of lattice strain along a stacking direction can consistently account for an upward jump of the close-packed interplanar spacing observed in course of the DHCP-to-FCC phase transition at about 500 K, contrasting with the downward atomic volume jump at this phase transition.

Quantitative analysis of basic parameters of the planar defects along with strain calculations is presented. The temperature evolution of stacking faults concentration and lattice strain in DHCP structure of La indicates on an equilibrium nature of the observed lattice imperfections rather then on a non-equilibrium one. Such an equilibrium microstructure can arise due to an additional gain in electronic energy, which stabilizes the DHCP lattice, at cost of elastic distortive energy [1]. The analysis of X-ray measurements complemented by TEM study shows that a partial relaxation of the induced short-range elastic stresses can proceed via incretion of stacking faults in DHCP structure of La.

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Keywords: metals, stacking faults, phase transitions and structure