

Nano-ball allophane is a naturally occurring aluminum silicate mineral with hollow spherical morphology. Diameter of the mineral is observed as 3.5 to 5.0 nm with TEM, and cation exchange experiments have proven the existence of some pores along the spherule wall. Chemical structure of the wall is similar to that of imogolite with nano-tube structure, where orthosilicates are bonded inside of gibbsite vacant site (imogolite sheet). However, whole chemical structure of the nano-ball has not been clarified. We succeeded to tentatively construct the whole chemical structure of the ball by assuming an expanded truncated octahedron composed of hexagonal imogolite sheets. By changing size of the imogolite sheets, diameters of the ball become 1.5 nm, 3.0 nm, 4.5 nm, and so on. Here we present full-structural optimization results for the nano-ball with diameter of 1.5 nm. Gaussian 03 for UNIX revision C.01 with HF/6-31G(d) method was used for calculations. The 6-coordinated Al and the 4-coordinated Si atom in the optimized structure were stable and no change in its ball shape structure. The calculated O · · · O atom distance in the vacant octahedral site that is substituted with orthosilicate has average 2.62 Å. Meanwhile, in the outer vacant octahedral sheet, the distance has average value of 4.25 Å for. It can be said that these contractions from substituted Si atom cause transformation of a planar gibbsite sheet to a material with spherical shape. Until now, there are no reports on the evidence of smallest nano-ball allophane except with diameter of 3.5 to 5.0 nm. However, our calculation result confirmed that the smallest of nano-ball allophane is stable and possible exists in the soil natural environmental.

Keywords: nano-ball allophane, *ab initio*, perfect mineral

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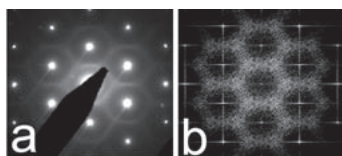
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Crystal structures and diffuse scattering of compounds with graphite-like (B,C)-nets

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The crystal structures of the new compounds Ca(B,C)₆ (hexagonal, $a = 4.563(1)\text{Å}$, $c = 4.396(1)\text{Å}$) and Ca(B,C)₈ (hexagonal, $a = 2.588(1)\text{Å}$, $c = 4.434(1)\text{Å}$) were determined from powder diffraction data. The compounds consist of planar graphite-like (B,C)-nets, intercalated by calcium atoms. In Ca(B,C)₆ one third of the hexagonal prismatic voids formed by the (B,C)-layers is occupied by Ca. In Ca(B,C)₈ the Ca-atoms are disordered, which gives rise to honeycomb-like diffuse scattering visible in the electron diffraction pattern (Fig. 1a). A model for the calcium distribution was developed and the diffuse scattering could be simulated successfully with the program DISCUS [1] (Fig. 1b).

[1] Proffen T., T., J. Appl. Cryst., 1997, 30, 171



Keywords: diffuse diffraction, powder diffraction, intercalation chemistry

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Synthesis and crystal structure of some indole derivatives complexes

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Schiff bases of hydrazone derivatives were synthesized from a condensation reaction involving hydrazones or amines and carbonyl containing compounds via reflux in ethanol for several hours. The crystal structure of the some complexes has different topology such as C18H20N8S2Ni which has a layer structure.

Keywords: indole, complexes, layer structure

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Preparation of ferrites MFe₂O₄ (M=Co,Ni) nanoporous ribbons structure and their magnetic properties

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Spinel ferrites, MFe₂O₄ (M=Co, Ni), ribbons with nanoporous structure were prepared by electrospinning combined with sol-gel technology. The ribbons were formed through the agglomeration of magnetic nanoparticles with PVP as structure directing template. The length of the polycrystalline ribbons can reach several hundred micrometers and the width of the ribbons can be tuned from several micrometers to several hundred nanometers by changing the concentration of precursor. Nanoporous structure was formed during the decomposition of PVP and inorganic salts. The ribbons exhibited weak saturation magnetizations and low coercivities at room temperature, but at low temperature, saturation magnetizations and coercivities increased a lot, especially for CoFe₂O₄ ribbons, reaching to 72 emu/g and 1.45 T at 2 K respectively. These novel magnetic ribbons can potentially be used in micro/nano electronic devices, magnetic sensors and flexible magnets.

Keywords: synthesis inorganic, magnetic oxides, ferrites

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Controllable synthesis and properties of ferric oxide nanostructural materials

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The design and synthesis of nanostructural materials have been among the important research topics of nanoscience due to their

unique structure, size and shape-dependent phenomena. Therefore, systematic directions for synthetic methods and an understanding of the mechanisms by which the structure, size and shape of the nanostructural material can be controlled are of particular interest. In this work, we report the controllable synthesis of ferric oxide nanostructural materials utilizing a simple hydrothermal method. We also examine the roles of parameters critical to the size and shape guiding processes and properties of the synthesized nanostructural materials. In a typical synthesis, added the ferric solution and additive to NaOH solution with various concentrations under vigorous magnetic stirring, and then transfer the mixture to a stainless steel autoclave. The products were characterized by XRD, SEM, TEM, ED, IR, TG-DTA, and SQUID. The XRD patterns of the as-prepared products were shown that, all of the peaks can be easily indexed as the rhombohedral α -Fe₂O₃. The SEM images indicate all products are composed of a large number of individual nanoparticles. The structure, size and shape of nanostructures could be control by adjusting hydrothermal conditions.

Keywords: hydrothermal synthesis, ferric oxide, nanostructural materials

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Growth and characterization of Nd_{1.85}Ce_{0.15}CuO₄ samples

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Recently several attempts have been made of looking at the physics of electron-doped and hole-doped cuprates under a unifying point of view, possibly elucidating the general mechanism for high-T_c superconductivity [1]. The fabrication method of Nd_{1.85}Ce_{0.15}CuO₄ bulk samples, based on a systematic control of the microstructural and phase homogeneity, is of fundamental importance in order to obtain sintered targets and precursors for high quality thin films and single crystals fabrication, respectively. Structural and electrical characterization of samples fabricated in different ways (bulk, films and single crystals) as a function of growth conditions and thermal treatments will be presented. We investigated morphology and composition by Scanning Electron Microscopy, Energy Dispersive Spectroscopy and Wavelength Dispersive Spectroscopy to verify the right stoichiometry, the presence of spurious elements, clusters and undesired phases. High resolution x-ray diffraction allowed to measure the structural parameters and to detect possible different phases and grain orientations. Standard four-probe resistance versus temperature measurements have been performed to study the transport properties of all the samples. Moreover, x-ray excited photoemission experiments performed at the European Synchrotron Radiation Facility have been used for obtaining information on the electronic configuration of the superconducting state as well as in the normal state [2,3].

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 [2] G. Panaccione et al., Phys. Rev. B 77, 125133 (2008).
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Keywords: superconducting oxides, X-ray techniques, resistivity

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Crystal structure and superconducting properties of monoclinic perovskite BaPb_{0.7-x}Sb_xBi_{0.3}O₃

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Starting materials BaCO₃, PbO₂, Bi₂O₃ and Sb₂O₅ were pressed into pellets and sintered in slowly flowing oxygen at the temperature of 1123 K for 15 hours. Polycrystalline BaPb_{0.7-x}Sb_xBi_{0.3}O₃ pellets were powdered. X-ray diffraction analysis was performed at room temperature using Siemens D5000 X-ray Powder Diffractometer with K α radiation. The space group was determined to be *I*2/*m* (No. 12), which was the same as for BaPbO₃ [1]. The lattice parameters were calculated using Powder Cell for Windows program [2]. The upper limit of lead replacement by antimony in monoclinic BaPb_{0.7-x}Sb_xBi_{0.3}O₃ was found to be $x = 0.4$. The lattice parameters *a*, *c* and the volume of the unit cell decrease with increasing *x* parameter up to $x = 0.2$. Then increasing the *a* and *c* lattice parameters and the volume of the unit cell in the *x* range $0.2 < x < 0.4$ is observed. The *b* lattice parameter decreases with increasing *x* parameter in the whole examined range. The monoclinic angle beta corresponds to the angle between the cubic directions [110] and [1-11]. Electrical resistivity measurements were performed to examine superconducting properties of the samples. Maximum transition temperature T_c equal to 13.2 was reached for the $x = 0.2$. The minimum of the unit cell volume in the BaPb_{0.7-x}Sb_xBi_{0.3}O₃ system is also observed for the $x = 0.2$. Oxygen deficiency leads to a loss of superconducting properties and change in the space group. Semiconductor BaPb_{0.7-x}Sb_xBi_{0.3}O_{3-d} compounds have space group *I*4/*mcm* at room temperature.

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Keywords: superconducting oxides, perovskites, resistivity

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Role of O atom modulation in the self-doped spin-ladder compound Sr₁₄Cu₂₄O₄₁

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The Sr_{14-x}(Ca, La, Y)_xCu₂₄O₄₁ series are so-called spin-ladder compounds with two-legged Cu₂O₃ ladder and one-dimensional CuO₂ chain. Especially, Sr_{14-x}Ca_xCu₂₄O₄₁ series form a self-doped system, because the formal valence of Cu is +2.25. The ternary Sr₁₄Cu₂₄O₄₁ as the parent material of Sr_{14-x}(Ca, La, Y)_xCu₂₄O₄₁ forms incommensurate composite crystal structure with the CuO₂ subsystem and the Cu₂O₃ subsystem. After modulated structure analysis with the BVS calculations of Sr₁₄Cu₂₄O₄₁, it has become apparent that most of the holes are located in the CuO₂ chain. The valence of Cu atoms in the ladder and the chain are well