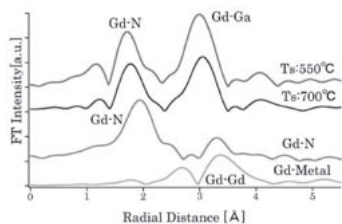


P16.06.43*Acta Cryst.* (2008). A64, C593**Crystal growth condition dependence of local structure around Gd in GaN nanotods**

Shuichi Emura, Hiroshi Kameoka, Hiroyuki Tambo, Yi-Kai Zhou, Shigehiko Hasegawa, Hajime Asahi

Osaka University, The Institute of Scientific and Industrial Research, Mihoga-oka 8-1, Ibaraki, Osaka, 567-0047, Japan, E-mail : emura@sanken.osaka-u.ac.jp

III-V semiconductors doped rare earth elements are attractive materials as magnetic semiconductors. They have high potential for applications in spin-dependent photonic and spintronics devices because of room temperature ferromagnetic behaviors. Here, we examine nanorods of GaGdN because nanorods are much better than film from crystallization and ferromagnetic points of view. Gd doped GaN nanorods were grown on naturally oxidized surfaces of Si (001) by radio-frequency plasma assisted molecular beam epitaxy. The substrate temperatures were set at 823K and 973K and Gd Cell temperature at 1373K. In order to study the local structure around Gd atoms in GaGdN nanorods, we observed XAFS spectra. Fig. 1 represents the radius structure functions (RSF) of GaGdN nanorods, which are analyzed from XAFS spectra. GdN and Gd-metal spectra are inserted in Figure 1 to compare GaGdN nanorod spectra. The peak, which is observed at 0.18 nm, corresponds to the Gd-N bond distance and at 0.31 nm corresponds to the Gd-Ga bond distance. Obviously, the RSFs of GaGdN are different from those of GdN and Gd-metal as shown in Fig. 1. Therefore, Gd ions are substituted at the Ga lattice points in GaGdN nanorods.



Keywords: diluted magnetic semiconductors, XAFS, rare earth element

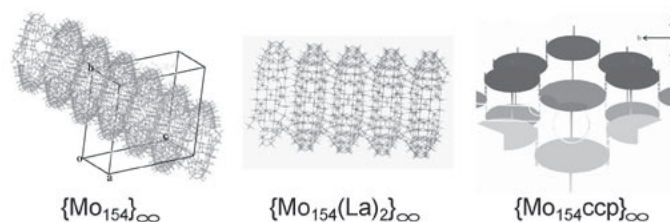
P16.08.44*Acta Cryst.* (2008). A64, C593**Photoinduced self-assembly to tube, chain, and other aggregate of molybdenum-blue nano-rings**

Toshihiro Yamase, Petra Prokop, Minako Iwatani, Eri Ishikawa

Tokyo Institute of Technology, Chemical Resources Laboratory, R1-21 4259 Nagatsuta, Midori-ku, Yokohama, Kanagawa, 226-8503, Japan, E-mail : tyamase@res.titech.ac.jp

The prolonged photolysis of aqueous solutions containing $[Mo_{36}O_{112}(H_2O)_{16}]^{8-}$ ($\{Mo_{36}\}$) and electron donors at pH=1 with or without lanthanide ions (Ln^{3+}) led to the formation of a variety of aggregates of the car-tire-shaped Mo-blue nano-rings with outer and inner ring-diameters of 3.5 and 2.2 nm, and 1.1-nm thickness. Structures of tube, $[Mo_{28}^{V}Mo_{126}^{VI}O_{446}(OH)_{12}(H_2O)_{66}]^{8-}$ ($\{Mo_{154}\}$), chain, $[MoV_{28}MoVI_{118}O_{424}(OH)_{20}(H_2O)_{60}\{Ln(H_2O)_5\}_2]^{10-}$ ($\{Mo_{146}Ln_2\}$) ($Ln = La, Er$), and cubic-close-packing (ccp)-like aggregate, $[MoV_{28}MoVI_{126}O_{424}(OH)_{40}(H_2O)_{62}]^{16-}$ ($\{Mo_{154}ccp\}$), were x-ray crystallographically characterized. The motif of the Mo-O-Mo linkage between inner rings in neighboring ring molecules is different among three structures: four *head-to-linker* and two *linker-to-linker* linkages for $\{Mo_{154}\}$, two *linker-to-edge* for $\{Mo_{146}(Ln)_2\}$, and two *linker-to-linker* for $\{Mo_{154}ccp\}$. The incorporation of Ln^{3+} in the inner ring of $\{Mo_{146}Ln_2\}$ suggests that Ln^{3+} is involved in the dehydrative condensation between inner rings of Mo-blues to yield aggregates

which let us expect promising properties in the nanostructure landscape for material science.



Keywords: photoinduced self-assembly, nano-tube and -chain, molybdenum-blue nanorings

P16.10.45*Acta Cryst.* (2008). A64, C593**On the nature of crystal growth units**

Askhab M. Askhabov

Institute of Geology Komi Science Centre Uralian Branch of Russian Academy of Sciences, xmin@geo.komisc.ru, Syktyvkar, Komi Republic, 167982, Russia, E-mail : xmin@geo.komisc.ru

The problem of how the crystals grow, was, in general, solved by mid part of the past century. However, debates about the nature of the building units at crystals growing continue hitherto. The key ideas are the following: 1. The crystals grow by joining separate atoms (ions) or molecules. 2. The building units at crystals growing are separate crystalline blocks. In principal, realization of these two extreme variants does not disagree with the general laws of physics and chemistry. In fact, majority of the modern theoretical models of the crystals growing is modeled on their base. With that, another idea – on the building units as particles of larger ones, than separate atoms (molecules), but not being crystalline particles - has already long been discussed and finds all more pieces of experimental verification. The most spreading ideas are: 1. On non-Kossel crystal growth (L.N.Rashkovich et al.). 2. On aggregation of crystals from polyhedral structural units (G.D.Ilyushin et al.). 3. On specific pre-crystallization nano-clusters of “hidden” phase (quaterons) as of basic units of the growth (A.M.Askhabov). Each of these new ideas, solving one and the same problem - on the nature of the building units - differently, turned out to be exceedingly fruitful for making clear the mechanism of real crystal formation. As a result we have to revise a number of the outdated ideas on the crystal growth. In the presentation the basic ideas on the quateron mechanism of the crystal growth are discussed and comparative analysis of the specified above new ideas on the nature of the building units, the mechanism of their formation, the forms of existence and their role in the process of growth are given. This study was supported by RFBR (08-05-00346a) and Scientific School (3266.2008.5).

Keywords: crystal growth, growth units, nano-clusters

P16.14.46*Acta Cryst.* (2008). A64, C593–594**Polymorphism below room temperature**

Dmitry S. Yufit, Judith A.K. Howard

University of Durham, Chemistry, South Rd., Durham, Durham, DH1 3LE, UK, E-mail : d.s.yufit@durham.ac.uk

The crystals of new polymorphic modifications of some common

Poster Sessions

solvents were grown in situ on a diffractometer from a mixture of two or more liquid at ambient conditions compounds and structurally characterized. This method, pioneered in [1], differs from standard in situ crystallization technique as crystallization from melt differs from solution crystallization and may produce different polymorphs. The structures of new polymorphs of several compounds (cyclobutanone, ethylacetate, butanone) were obtained by this method. Their molecular structures and packing of molecules are described and compared with those of known polymorphs of the same or similar compounds. The intermolecular interactions determining the packing of molecules are analysed by various methods as well as possible factors affecting the packing. The technical details of experimental setup and data processing are discussed as well.

I. J. Bennet-Buchholz, T. Haumann, R. Boese; J. Chem. Soc. Chem. Commun., 1998, 2003-2004

Keywords: low-melting compounds, polymorphic structures, crystal growth

P16.03.47

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Hydrothermal synthesis of (K,Na)NbO₃

Albertus D. Handoko, Gregory K.L. Goh

Institute of Materials Research and Engineering, Materials Growth, 3 Research Link, Singapore, Singapore, 117602, Singapore, E-mail: ad-handoko@imre.a-star.edu.sg

Lead-free perovskite KNbO₃-based solid solutions can exhibit piezoelectric properties comparable to that of actuator grade lead zirconate titanate piezoelectrics in the vicinity of the morphotropic phase boundary. Conventional high temperature processing of KNbO₃-based solid solution involves energy intensive and laborious processes with risk of getting non-stoichiometric compound due to potassium volatilization. In this study, crystalline (K,Na)NbO₃ solid solutions are synthesized hydrothermally at significantly lower temperature of 200 °C for the first time close to the morphotropic phase boundary by using a mixed NaOH and KOH solution. Above a certain critical ratio of NaOH to KOH concentration, a secondary NaNbO₃ perovskite phase always formed alongside the solid solution. Details of NKN phase formation, structural and composition in soft chemistry solution route were studied, including presence of different intermediate phases which potentially be technical barrier to synthesize pure NKN phase using single step hydrothermal synthesis. Despite this difficulty, a short 2 hour heat treatment at 800 °C was successfully used to convert the mixture of (K,Na)NbO₃ and NaNbO₃ powder to a single solid solution phase powder close to the morphotropic phase boundary. This opened a new possibility of reducing energy requirement in NKN powder compact synthesis via solid state reaction.

Keywords: hydrothermal synthesis, sodium potassium niobate, ferroelectric materials

P16.03.48

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Perovskite-type LnFeO₃ (Ln= Y, Pr, Nd, Sm, Gd, Tb, Dy, Ho) prepared by mild hydrothermal method

Shouhua Feng¹, Ganghua Zhang², Hongming Yuan³, Meiqi Yang⁴, Yan Chen⁵, Shijing Zhang⁶

¹Jilin University, College of Chemistry, JILIN UNIVERSITY State Key Laboratory of Inorganic Synthesis and Preparative Chemistry 2699

Qianjin Street, Changchun 130012 P.R.China, ChangChun, JiLin, 0431, China, ²zhangjiesss923@sohu.com, ³hmyuan@mail.jlu.edu.cn, ⁴largeface622@126.com, ⁵chenyanjlu@yahoo.com.cn, ⁶janejian80@163.com, E-mail: shfeng@mail.jlu.edu.cn

A series of the rare-earth orthoferrites LnFeO₃ (Ln= Y, Pr, Nd, Sm, Gd, Tb, Dy and Ho) that were characterized by powder X-ray diffraction with the orthorhombic perovskite lattice symmetry have been prepared under mild hydrothermal conditions. In hydrothermal processing of these materials it is found that their formation are mainly affected by the reaction temperatures, times, and appropriate alkaline solution range for different lanthanide elements, while the particle sizes of the samples which are applied to image by means of scanning electron microscopy vary significantly with the amount of OH⁻ anions in the reaction systems.

Keywords: hydrothermal, perovskite, orthoferrites

P16.03.49

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Effect of anion adsorption on the hydrothermal growth of boehmite

Taobo He, Lan Xiang, Shenlin Zhu

Department of Chemical Engineering, Tsinghua University, Beijing, Beijing, 100084, China, E-mail: htb05@mails.tsinghua.edu.cn

The effect of the adsorption of the anions as nitrate, chloride and sulfate on the hydrothermal growth of boehmite (AlOOH) was investigated in this paper. The experimental results indicated that boehmite nano-flakes with a width of about 50 nm and boehmite nano-fibres with a preferential growth along [100] were formed after hydrothermal treatment (240 °C, 16h) of the freshly precipitated alumina gel at pH=10.5 and pH=4.0, respectively. The anions were difficult to be adsorbed on the boehmite surface under alkaline condition, thus had little influence on the hydrothermal formation of the corresponding boehmite nano-flakes. The formation of the boehmite nano-fibres was promoted by the adsorption of the anions on boehmite surface under acidic condition, and the increase of the aspect ratio of the nano-fibres was identical with the adsorption tendency of the anions (nitrate < chloride < sulfate).

Keywords: hydrothermal, boehmite, anions

P16.10.50

Acta Cryst. (2008). A64, C594-595

Using of Taguchi method for experimental design of crystallization processes of inorganic compounds

Shahriare Ghamamy, Monir Rahnam

Imam Khomeini International University, Chemistry, Imam khomeini International University, Noroozian street, Qazvin,, Qazvin, 34146-16818, Iran, E-mail: shghamami@yahoo.com

Taguchi design of experiments (DOE) method has been used for to plan a minimum number of experiments and optimization of crystallization processes. This method decrease the number of experiment that need to received to good crystals. Taguchi method can be designed for a wide range of specific functions. Using a special orthogonal array only a small set from all the possible experiment is selected. The simultaneous variation of the main crystallization parameters and their interaction were investigated using orthogonal array techniques. The relative magnitude of the effect of different