

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

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A series of the rare-earth orthoferrites LnFeO_3 (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

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Hydrothermal synthesis of $(\text{K},\text{Na})\text{NbO}_3$

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Lead-free perovskite KNbO_3 -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 KNbO_3 -based solid solution involves energy intensive and laborious processes with risk of getting non-stoichiometric compound due to potassium volatilization. In this study, crystalline $(\text{K},\text{Na})\text{NbO}_3$ 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 NaNbO_3 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 $(\text{K},\text{Na})\text{NbO}_3$ and NaNbO_3 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

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Perovskite-type LnFeO_3 (Ln = Y, Pr, Nd, Sm, Gd, Tb, Dy, Ho) prepared by mild hydrothermal method

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Effect of anion adsorption on the hydrothermal growth of boehmite

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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

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

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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