

Inflation rules are not only a way to characterize the self-similarity of aperiodic structures (that is, tilings or patterns), but they are also used as a tool to construct yet unknown structures. The latter, however, has applied mainly to low-dimensional cases, while the use has been scarcely explored for three-dimensional icosahedral quasilattices (IQL's). In this paper, we make use of point inflation rules (PIR's) [1] for generating various IQL's of all the three Bravais classes (P, F and I-types). A PIR operates on a point set as firstly expand it by a scaling ratio of the underlying Z-module and secondly replace every point by an icosahedral cluster which is the prototype of the IQL. The Bravais class of the IQL is determined by the prototype cluster and the scaling ratio. It is a natural consequence of the method that the IQL will have a dense packing of the prototype clusters, while the atomic surface tends to exhibit a fractal boundary. [1,2] Note that the arrangement of the clusters are not based on any of the tiling models (e.g., the Ammann rhombohedral tiling). An extension of the method is presented where several different prototype clusters are used. Such an extension corresponds to introducing several different atomic surfaces on different special points of the six-dimensional icosahedral lattice. The widened range of IQL's that can be generated contains possible candidates that may be used for modeling real quasicrystals. [1] K. Niizeki, *J. Phys. A: Math. Theor.* 41 (2008), in print. [2] N. Fujita and K. Niizeki, *Phil. Mag.* (2008), in print.

Keywords: quasicrystal crystallography, theoretical structure modelling, aperiodic structures

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Study of stoichiometric glass ceramics formation in the BaO-Bi₂O₃-B₂O₃ system

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Interest to BaO-Bi₂O₃-B₂O₃ system is connected to revealing new passive and active functional glasses and glass ceramics(GC). This system isn't investigated enough and its phase diagram is absent. The incongruent melted at 754°C ternary BaBiBO₄ compound was synthesized and characterized recently by the solid-state sintering. Three ternary compounds were revealed in this system: congruent melted BaBi₂B₄O₁₀(730°C) and BaBiB₁₁O₁₉(807°C) compounds and Ba₃BiB₃O₉ compound which has phase transition at 850°C and subsequent solid state decomposition at 885°C. In the present work our attention has been concentrated on the study of stoichiometric ternary borates glass forming ability and the GC availability on their basis and the formed crystals characterization. The batches of all testing compositions were prepared from chemically pure grade reagents and were melted in quartz crucibles at 900-1000°C in electrical furnace. Due to chemical analysis SiO₂ transition in glass melts at melting didn't exceed 2 wt. %. All compounds have good glass forming ability and form stable glasses. The temperature intervals and character of synthesized glasses crystallization and m.p. of formed crystals have been revealed from the DTA curves. Regimes of powder and bulk glass samples crystallization are studied and products of their crystallization are identified by X-ray analysis. The studies have shown that all stoichiometric glass basis are perspective for the GC with different functionality development: crystallized frits with high resistivity for packaging or covering on the ceramic or

metallic plates; transparent nonlinear-optical GC.

Keywords: barium bismuth borate compounds, glass ceramics, stoichiometric glass basis

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Transparent glass-ceramics containing lead fluoride crystals

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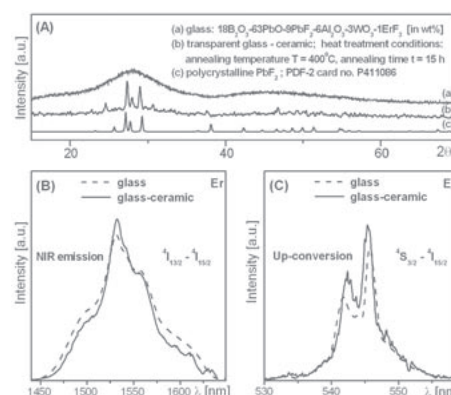
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Transparent glass-ceramics (TGC) as new host materials for rare earths have a great deal of interest due to their unique behavior like fluoride nanocrystals in oxide glass matrices. Heat treatment introduces transformation from glass to glass-ceramic, causing changes in spectroscopic properties like: narrowing of spectral lines and elongation in lifetimes of fluorescent states. Er-doped lead borate glasses before and after annealing were investigated using X-ray diffraction and luminescence spectroscopy. They present interesting spectroscopic properties in relation to NIR emission and up-conversion applications [1]. During heat treatment, TGC systems were obtained. Phase identification reveals, that crystalline peaks can be related to the orthorhombic lead fluoride phase, in contrast to other TGC systems containing cubic lead fluoride crystals [2].

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References

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Keywords: glass-ceramics, X-ray diffraction, luminescence spectroscopy

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Influence of starting materials on hydrothermal synthesis of six-pointed starlike anatase aggregates

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Six-pointed starlike anatase aggregates were hydrothermally synthesized from aqueous mixtures of titanium tetraisopropoxide and tetramethylammonium hydroxide (TMAOH). It is noteworthy that though anatase has a tetragonal lattice, the anatase aggregates

has a six-pointed starlike shape like ones of hexagonal crystals. We recently examined the structures of the titanium species in the starting solutions and the starlike aggregates. The starting solutions were transparent aqueous ones of crystalline titanate colloids having a layered lepidocrocite-type structure. The starlike aggregates consisted of acicular anatase crystals elongated along the *c*-axis. The acicular crystals were assembled by oriented attachment and twinning on the {112} planes, to form an arm of the aggregates. The fact that the angle between (112) and (11-2) is about 60° contributes to the six-fold symmetry of the starlike aggregates. In this study, the influence of the type of the tetraalkylammonium hydroxide on the formation of the starlike aggregates was examined in order to elucidate the formation mechanism of the aggregates. TMAOH, N(C₂H₅)₄OH (TEAOH), N(C₃H₇)₄OH (TPAOH) and N(C₄H₉)₄OH (TBAOH) were used as the alkylammonium hydroxide. The use of TMAOH and TEAOH led to the formation of a large number of starlike aggregates. On the other hand, the use of TPAOH and TBAOH decreased the number of the starlike aggregates. It is known that the intercalation of TPA⁺ and TBA⁺ ions into the interlayer of the lepidocrocite-type titanate leads to exfoliation of the titanate layers. Thus, it is inferred that the layered structure of the colloids in the starting solutions plays an important role in the formation of the six-pointed starlike anatase aggregates.

Keywords: titanium oxide compounds, hydrothermal synthesis, aggregates

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A systematic study of the crystal structures of monomethine cyanine dyes

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Cyanines are an important class of dyes which are known for their spectral sensitisation properties and various technical applications. Many of their spectral properties arise from their ability to form aggregates in both solution and on surfaces for which a large number of studies have been made. However there is little information concerning their solid crystalline forms; indeed relatively few examples of their structures are known. For example, in the current version of the CSD there is only one monomethine dye with a simple counterion (Br⁻). We have made a systematic study of a series of monomethine crystal structures and present here a survey of their similarities, trends and differences.

Keywords: crystal systematic, dyes, packing analysis

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Growth and characterization of new nonlinear optical crystals L-valine and L-valine hydrobromide

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The growth of a new nonlinear optical material L-valine and its inorganic complex L-valine hydrobromide (VHBr) are reported

here. The grown crystals were characterized by FTIR, single crystal XRD, DTA-TGA, DSC, optical transmission and second harmonic generation (SHG) efficiency measurement. Bulk single crystals of L-valine and VHBr were grown from their aqueous solution by solvent evaporation method at constant temperature 28°C and 35°C respectively. Single crystal XRD of L-valine and VHBr reveals the lattice parameters to be $a = 9.701(3)\text{Å}$, $b = 5.261(2)\text{Å}$, $c = 11.953(2)\text{Å}$ and $\beta = 90.66^\circ(1)$ for L-valine and $a = 10.154(2)\text{Å}$, $b = 7.415(2)\text{Å}$, $c = 5.333(2)\text{Å}$, and $\beta = 91.22^\circ(2)$ for VHBr. The result of DTA-TGA study indicates that there is no water of crystallization present in either of the samples. DSC study shows the possibility of phase transition in VHBr. Both the crystals of L-valine and VHBr are optically transparent in the UV-Vis-NIR region with 80% transmission for L-valine and 100% transmission for VHBr. Lower percentage of transmission for crystals of L-valine may be due to poor crystal quality in comparison to VHBr. The second harmonic efficiency of L-valine is 0.82 times that of KDP where as that of VHBr is found comparable to Urea. The above discussion reveals that both L-valine and its derivative VHBr can be used effectively as a new nonlinear optical materials, but the SHG efficiency of VHBr is much higher than that of L-valine. Though L-valine is thermally more stable than VHBr but VHBr is optically more transparent than L-valine as the crystals are superior. The crystals of VHBr are more readily obtained than that of L-valine. Lastly, a probability of phase transition made VHBr a very interesting new NLO material.

Keywords: nonlinear optical materials, crystal growth from solution, characterization

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Powder X-ray diffraction of stacking fault containing β -FeSi₂

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β -FeSi₂ has been studied as thermoelectric materials and optoelectric semiconductor materials. We noticed that the intensities of some specific diffraction peaks were smaller than those calculated with the structure parameters determined by single crystal XRD. We prepared β -FeSi₂ from a mixture of Fe and Si at 873-1173 K by using a Na. The powder XRD patterns of the samples were compared with the patterns calculated with DIFFaX for the crystals containing stacking faults. The small diffraction intensities were caused by stacking faults.

Keywords: powder X-ray diffraction, thermoelectric materials, stacking faults in inorganic structures

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The doubly non-commensurate structure of synthetic tin-selenium cylindrite

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