selective substitution of Fe for Mn. From magnetic measurements a general increase of the magnetic ordering temperature with increasing x, as well as multi and single-phase magnetic behaviour, is observed. A correlation with the crystal structure will be given.

Keywords: mixed-valence oxides, XRD, XAS

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Cellular Automata Modeling of Complex Inorganic Crystal Structures Sergey V. Krivovichev[a], Vladislav V. Gurzhiy[a], Ivan G. Tananaev[b], Boris F. Myasoedov[b]
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Cellular automata (CA) have been introduced for simulation of self-reproductive biological systems [1] and have attracted considerable attention as a possible environment for modeling of a broad range of physical objects and processes [2], in particular, of periodic growth of complex chemical structures [3, 4]. From the formal point of view, CA is defined as a collection of five basic components:
CA := <Z, S, N, f, B>,
where Z is a lattice (discrete working space of the CA consisting of cells; the simplest example is a 2-D plane filled by square cells);
S = {0, 1, 2, ...} is a finite number of values that the cells may take (usually, these values are associated with colors, e.g. S = {0, 1} characterizes a binary (2-color) CA;
N = {$-k_1$, $-k_1$+1, ..., -1, 0, 1, ..., k_2-1, k_2} is a neighborhood of CA action (for 1-D CA the value of the cell x_0 at the time t = 1 is determined by the values of k_1 and k_2 cells on the left and right sides at the time t = 0 (in simplest case, the neighborhood is symmetrical k_1 = k_2 = 1 and has a radius k_0 = 1, i.e. it consists of three cells (k = 3): x_{-1}, x_0, x_1; the value of the cell x_0 at the time t = 1 is determined by the values x_{-1}, x_0, x_1 at the time t = 0);
f is a local transition function that works for a certain neighborhood (usually written as a set of rules of the form 010 $\rightarrow$ 1;
B is a boundary conditions.
Since crystal structures are periodic by definition, their growth and topology can be described using a special class of CA that produce repetitive patterns.
In this contribution, we will construct CA models of such various classes of inorganic structures as uranyl selenates and iron sulfides. One of remarkable results of CA applications in crystal chemistry is that *the same* CA may generate *different* structural topologies. The resulting topology is determined by the initial conditions, i.e. by the structure of the first row. In the language of chemistry, this means that molecular-level growth mechanism of uranyl selenate layers is the same and the topology of the structure is controlled by the structure of nucleus spontaneously formed in solution.
In addition, application of CAs allows to predict possible topologies that may form in specific system. It also provides a computational basis for studying complexity and dynamics of topologically and chemically similar structures forming under similar physico-chemical conditions.
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Keywords: cellular automata, structure topology, uranyl selenates

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Elastic anomalies and precursor effects in CBN and Ce:CBN relaxor ferroelectrics. Chandra Shekhar Pandey[a], Jürgen Schreuer[a], Manfred Burianek[b], Manfred Mühlberg[b]. [a]*Institut für Geologie, Mineralogie und Geophysik, Ruhr-Universität Bochum, Germany.* [b]*Institut für Krystallographie, Universität zu Köln, Germany.*
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Ferroelectric materials are widely investigated because of their often promising electro-optic, pyroelectric, piezoelectric and photorefractive properties. $Ca_xBa_{1-x}Nb_2O_6$ (CBN-x) and cerium doped $Ca_xBa_{1-x}Nb_2O_6$ (Ce:CBN-x), both relaxor ferroelectric materials crystallizing in the partially filled tetragonal tungsten bronze (TTB) structure type, provide excellent alternatives to strontium barium niobate (SBN) for device applications because of their relatively high Curie temperature (T_C = 264°C for x = 0.28 for undoped and T_C = 200°C for Ce-doped CBN with x = 0.28).
Here we report on the anomalous elastic behaviour and precursor effects of undoped CBN-28 and Ce:CBN-28 single crystals grown by the Czochralski method as determined between room temperature and 1323 K employing resonant ultrasonic spectroscopy (RUS).
The temperature evolution of the elastic constants c_{ij} in the paraelectric phase (point symmetry group 4/mm) of Ce:CBN-x shows pronounced anomalies like in undoped CBN-28 [1]. Doping with Ce leads to a stiffening of all elastic constants of CBN-28. Below about 900 K all resonances of the freely vibrating samples show rapid softening when approaching T_C. The onset of elastic softening is frequency dependent. The deviations from Cauchy relations indicate predominance of ionic bonding at high temperatures. When approaching T_C directional bonding contributions become more and more important along the tetragonal axis. In the ferroelectric phase strong ultrasound dissipation effects appear which are probably related to interactions between sound waves and ferroelectric domain walls.

[1] Pandey C. S., Schreuer J., Burianek M. and Mühlberg M., *Phys. Rev. B* submitted (part of the manuscript was presented on ISAF-2009 held at Xian, China).

Keywords: calcium barium niobate, ferroelectric transition, elasticity