PS10.04.13 SYMMETRY RELATIONSHIPS IN THE HOMEOTYPICAL ALUMINUM-RICH STRUCTURES WITH PENTAGONAL CHANNELS. M. Ellner, U. Burkhardt and Yu. Grin(*), Max-Planck- Institut fur Metallforschung and Max-Planck-Institut fur Festkörperforschung (*), Stuttart, Germany

A significant feature of some homeotypical aluminum-rich structures with transition metals (TM) is the occurrence of finite or infinite pentagonal channels, which is dependent on chemical composition i.e. the stoichiometry of these intermetallic compounds is controlled by both s-, p-electrons of aluminum and d-electrons of TM. A phase bundle occurrs in the aluminum-rich portion of the binary system Co-Al: Co_2Al_5 (hP28, $P6_3/mmc$), $CoAl_3$, Co_4Al_{13}(h), m-Co_4Al_{13} (mC102-7.2, Cm) and o-Co_4Al_{13} (oP102, $Pmn2_1$). The homeotypical structures Co_2Al_5, mCo_4Al_{13} and o-Co_4Al_{13} show different arrangement of pentagonal channels.

Moreover, the structures o-Co_4Al_{13} and m-Co_4Al_{13} are formed by two flat (AA') and two puckered (BB') layers of atoms in the sequence ABA'B'. These structure types can be described in terms of pentagonal and rhombic clusters with dimensions d=4.7 Å and h=8.1 Å. The edges of the pentagonal clusters are formed by TM atoms. Two TM atoms are situated in the middle of the prisms at y = 0.25 and y = 0.75. Each of them is surrounded by five aluminum atoms in form of puckered pentagons. The basal faces of the prisms are alternate occupied by one aluminum atom or five aluminum atoms forming distorted pentagon.

A regular cyclical tiling of pentagonal clusters yields 2D motives either with pentagonal twins showing the point-group symmetry C_5 or with decagonal twins showing the point-group symmetry C_{10}. The unit cell of one segment of these motives is conform with the unit cell of the m-Co_4Al_{13} structure, while the twin-interface arrangement corresponds to a partial unit cell of o-Co_4Al_{13}.

Pentagonal and rhombic clusters probably dominate the structure $CoAl_3$. The structure proposal for $CoAl_3$ agrees well with the experimental powder diffraction data.

PS10.04.14 X-RAY DIFFUSE SCATTERING IN QUASICRYSTALS: COLLECTING LARGE 3-DIMENSIONAL DIFFRACTION VOLUMES WITH IMAGE PLATES Michael A. Estermann, Walter Steurer, Laboratory of Crystallography, ETH Zentrum, CH-8092 Zurich, Switzerland

Strategies for collecting and analysing diffuse scattering data of quasicrystalline materials will be presented: Automatic indexing of rotation pictures from aperiodic materials [1], background analysis in the presence of diffuse scattering, reconstruction of arbitrary slices and volumes in diffraction space and data reduction.

Diffuse scattering effects can be observed in most materials with decagonal or icosahedral diffraction symmetry. These effects cannot be explained by strict quasiperiodic ordering, various kinds of disorder must be considered, such as random static disorder or orientationally ordered nanodomain structures. The knowledge of the real structure of decagonal and icosahedral phases is an important step towards understanding their physical properties which are strongly determined by defects and disorder.

Our primary aim is to proceed towards a quantitative analysis of the disorder effects; a number of models based on the known average structure of decagonal AlCoNi are currently being developed in our laboratory.

To record quantitatively large volumes of X-ray diffraction space we use the MarResearch imaging plate detector system which is an on-line imaging plate scanner in combination with simple rotation geometry. Small rotation ranges of 0.2° or even still images result in 2D spherical sections which are small enough to allow a complete reconstruction of the diffraction space. After the usual corrections for resolution, absorption and Lp effects, the entire measurable reciprocal space is accessible for numerical calculations.

[1] M.A.Estermann & W.Steurer (1995). Proceedings of the 5th International Conference on Quasicrystals. Avignon, France. Editors: C. Janot & R Mosseri. World Scientific Publishing.

PS10.04.15 FIBONACCI CHAIN - A QUASIPERIODIC APPROACH OF ONE DIMENSIONAL APERIODIC STRUCTURES. Maria Farkas-Jahnke, Research Institute for Technical Physics of HAS, H-1325 Budapest P.O.Box 76, Hungary

In aperiodic lattices built up of translationnaly equivalent layers - for example lattices of closed packed structures containing many stacking faults - only short range order can be determined exactly. In ZnS lattices the rate of occurences of stackings up to five layers can be determined using the data of X-ray patterns of the singl crystals in question. The longer range order in these faulted crystals can be approached by Fibonacci-chains, whose elements are composed as suitable arrangements of these five layer structure elements. In this way, relatively good quasiperiodic description to a long sequence of the faulted lattice can be given which can be used for interpretation of the dependence of certain physical properties from different lattice fault configurations.

PS10.04.16 STRUCTURAL STUDIES ON INCOMMENSURATE-NORMAL PHASE TRANSITION IN Co-ÅKERMANITE, $Ca_2CoSi_2O_7$. K. Hagiya, K. Kusaka, N. Haga, M. Ohmasa and K. Iishi[1]. Department of Life Science, Himeji Institute of Technology, Japan; [1]Department of Mineralogical Science and Geology, Yamaguchi University, Japan

Since comparison between the structure of incommensurate phase and that of normal phase in the title compound is expected to be informative to elucidate origin of the modulation, the present studies on change of the structure at elevated temperatures have been carried out. Two-dimensional incommensurate phases of synthetic åkermanite solid solution $Ca_2(Mg,Fe)Si_2O_7$ were found by Hemingway *et al.*[1] and Seifert *et al.*[2] independently. They found that åkermanite undergoes a reversible phase transition from the low-temperature incommensurate phase to the high-temperature normal phase. The modulated structures of the Co-analogue ($Ca_2CoSi_2O_7$) was determined by us[3] based on the five-dimensional description. The results revealed that the modulation is caused by the shifts of the constituent atoms.

The specimen of the single crystal was synthesized by one of the authors (K.I.). Temperature dependence of intensities and that of the cell parameters were examined *in situ* to observe the change of the structure. A fragment of the sample was mounted in a small gas blow heating system installed on an Enraf-Nonius CAD-4 diffractometer. Mo$K\alpha$ radiation monochromatized by graphite was used for the measurements. The temperatures, varied from room temperature to 270°C with arbitrary steps, were estimated by a thermocouple to regulating the heating system. The intensities were corrected for Lorentz and polarization effects.

The intensity of the satellites steeply weakens to background level at about 220°C. In connection with the change, the *c*-axis contracts at the temperature range between 210°C to 230°C, while the *a*-axis expands and the volume of the cell is held almost constant. The structures at the temperature range were analyzed carefully to clarify those phenomena.

1) Hemingway *et al.* (1986). *Can. Mineral.* **24**, 425-434.
2) Seifert *et al.* (1987). *Phys. Chem. Minerals* **14**, 26-35.
3) Hagiya *et al.* (1993). *Acta Cryst.* **B49**, 172-179.