PS10.04.17 SIMULATIONS ON THE PHASE TRANSFORMATION OF DECAGONAL Al-Co-Ni TO ITS CRYSTALLINE APPROXIMANTS. Matthias Honal, Torsten Haibach and Walter Steurer, Laboratorium für Kristallographie, ETH Zentrum, CH-8092 Zurich, Switzerland.

Model calculations simulating the transformation from the decagonal phase to an crystalline nanodomain structure have been performed, in direct and reciprocal space, respectively.

Starting from an idealised structure model of decagonal $Al_{70}Co_{15}Ni_{15}$ [1], a purely geometrical mechanism is applied, leading to a patchwork-like arrangement of crystalline nanodomains [2]. This is achieved by slight uncorrelated displacements of the atoms. The resulting orientation of the different nanodomains is determined by the minimum total sum of atomic shifts.

Models with dimension 8000 * 8000 * 4 Å^3, including about $2 \cdot 10^6$ atoms, have been used for the calculations. Resolution and coherence parameters have been considered corresponding to experimental conditions.

The resulting nanodomain-structure reproduces quite well the experimental observations [3]. The characteristics of different nanodomain models will be discussed in direct space as well as in reciprocal space.

[1] Steurer, W., Haibach, T., Zhang, B., Kek, S., Lück, R.: *The Structure of* $Al_{70}Ni_{15}Co_{15}$. Acta Crystallogr. **B49** (1993) 661-675.
[2] Steurer, W., Honal, M. and Haibach, T.: *Mechanism of phase transformations in decagonal phases.* Proceedings of 5th International Conference on Quasicrystals ICQ95. Singapore - World Scientific (1995) in press.
[3] Kalning, M., Press, W., Kek, S.: *Investigation of Decagonal* $Al_{70}Co_{15}Ni_{15}$ *Single Crystals by Means of High-resolution Synchrotron X-ray Diffraction.* Phil. Mag. Lett. **71(6)** (1995) 341-349.

PS10.04.18 DYNAMICAL DIFFRACTION AND X-RAY STANDING WAVES FROM 2-FOLD REFLECTIONS IN THE QUASICRYSTAL AlPdMn Terrence Jach, National Institute of Standards and Technology, S. M. Thurgate, Murdoch U., Australia, Yi Zhang, R. Colella, Purdue U., S. Kycia, Cornell U., A. I. Goldman, Iowa State U., M. de Boissieu, M. Boudard, LTPCM/ENSEEG, France.

We have observed x-ray diffraction from the (420024) and (640046) reflections of an AlPdMn quasicrystal in the back-reflection Bragg geometry θ_B=90°. The rocking curves observed by scanning the energy of the synchrotron radiation possess widths close to the Darwin width expected in a dynamical theory. As a result, observation of the Kα fluorescence from the Al and the Lα fluorescence from the Pd atoms exhibits strong x-ray standing wave behavior, similar to that observed in crystalline materials. The data suggest a long range order of "quasiplanes" of specific elements, as seen by a "coherent position" which differs for the x-ray fluorescence from the Al and Pd atoms.

PS10.04.19 DISORDER AND DIFFUSE SCATTERING OF CHANNEL TYPE INCLUSION COMPOUNDS WITH PERHYDROTRIPHENYLENE. O. König[1], H.B. Bürgi[2], T. Armbruster[2], J. Hulliger[1], Institute of Inorg., Analyt. and Physical Chemistry, University of Berne, Switzerland[1], Laboratorium of Chem. and Miner. Crystallography, University of Berne, Switzerland[2]

Intensive diffuse scattering is observed for a series of new crystalline inclusion compounds of racemic perhydrotriphenylene (PHTP) [1]. In these compounds stacks of PHTP form channels along the unique c axis hosting linearly shaped donor (D) - acceptor (A) substituted π-systems as guests [2].

For such guests X-ray photographs show difffuse scattering concentrated in plans perpendicular to the channel axis. This is explained by an one dimensional translational order of guest molecules within each channel (c_{guest}) and a lack of translational order between different channels. The period c_{guest} almost always agrees with the assumption of close packing along the channels and, depending on the ratio c_{host}/c_{guest} both commensurate and incommensurate cocrystals have been found. For a few cases, satelite reflections superimposed onto the diffuse layers indicate some correlation between guest molecules in different channels.

Analysis of Bragg scattering of the commensurate system {1-(4-Nitrophenyl)piperazine}$\cdot${PHTP}$_5$ revealed a centrosymmetric space group (Cmcm) for the host lattice and a polar space group Cmc2$_1$ for the guest molecules implying a parallel alignment of 1-(4-Nitrophenyl)-piperazine dipoles in different channels. The mechanism responsible for parallel alignment of the dipole in different channels, which are 14 Å apart, is until now not understood.

[1] M. Farina, in Inclusion Compounds 2 (Eds.: J.L. Atwood, J.E.D. Davis, D.D. MacNicol), Academic Press, London 1984, 69-95;
[2] J. Hulliger, O. König, R. Hoss, Adv. Mater. 7 (1995), 719-721.

PS10.04.20 COMPARISON OF THE LOW-TEMPERATURE PHASE TRANSITIONS IN K_2CoCl_4 AND K_2ZnCl_4. J.Kusz, J.Warczewski, University of Silesia, Institute of Physics, ul. Uniwersytecka 4, PL-40007 Katowice, Poland, A. Pietraszko, Institute of Low Temperature and Structural Studies of the Polish Academy of Sciences, PL-50950 Wroclaw, Poland

K_2CoCl_4 and K_2ZnCl_4 belong to the A_2BX_4 group of the ferroelectric compounds revealing a sequence of phases starting from the high temperature paraelectric phase (Pmcn) through the incommensurate phase with the modulation vector $q= (1/3 - \delta) c^*$ to the commensurate phase with $q= 1/3c^*$ and to the low-temperature commensurate phase with $q_1= 1/3c^*$ and $q_2=1/2a^* +1/2b^*$. The theoretical expectations [1] suggest that for the compounds of this group the symmetry of the low-temperature phase should be monoclinic (C1c1).

Our measurements made down to 100 K on the X-Ray 4-circle diffractometer showed that there is both no deviation of the angle β from 90° and no anomalies of the lattice parameters in the low-temperature phase. The FWHM of the h0l-type reflections increases for K_2CoCl_4 below the transition temperature (142 K) [2], contrary to K_2ZnCl_4. This fact can be interpreted as a very small monoclinic deformation of the low-temperature commensurate phase.

Analysis of the reflection intensities (hkl and ikl) for K_2ZnCl_4 at 155 K and 105 K did not show any increase of the R_{eq} factor. It means, that there is no significant assymetry, that could confirm any monoclinicity of the low-temperature phase in this compound.

References
[1] Dvorak V. and R.Kind, Phys. Status Solidi (b), 107, K109 (1981).
[2] Kusz J., A. Pietraszko and J.Warczewski, Phase Transitions (1996), in press.