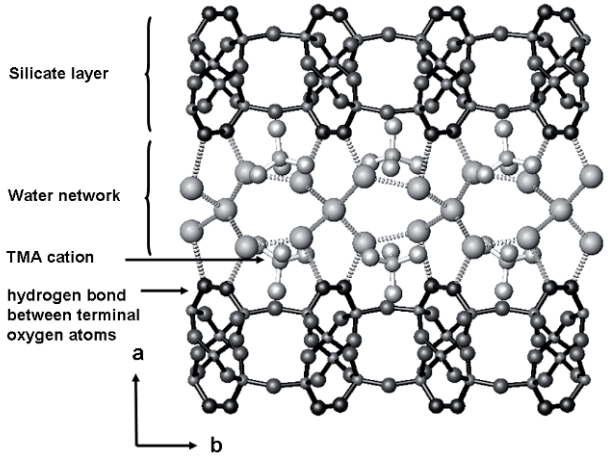
RUB-15-RT: Ic2a, $a_0$ = 27.905 Å, $b_0$ = 8.408 Å, $c_0$ =11.518 Å,
RUB-15-LT: I2, $a_0$ = 27.4376 Å, $b_0$ = 11.4032 Å, $c_0$ = 8.4138 Å,
β = 91.725°. The refinement converged to $R_{Bragg}$ = 4.1, $\chi^2$ = 2.4.

The structures of RUB-15-RT and RUB-15-LT differ only slightly: The powder diagram of monoclinic RUB-15-LT still shows the reflection conditions for the (pseudo-) symmetry Ic2a.




However, for the low temperature form it is possible to analyze the bonding system between water molecules, siloxane groups and silanol groups in more detail. The analysis of this bonding network revealed strong intra-layer hydrogen bonds between neighboring oxygen atoms of the terminal SiOH/$SiO^-$-groups. The analysis allowed to distinguish between Si-OH and Si-$O^-$-groups of the silicate layer showing additional strong hydrogen bonds bet-ween the Si-$O^-$-groups and water molecules of the water network.

The $^1$H NMR spectrum confirms the results of the X-ray structure analysis. It displays a broad signal at 3.4 ppm attributed to the protons of the TMA cation and of the water network, and a signal at 16.4 ppm corresponding to strong hydrogen bonds with an O…O distance of about 2.4 Å.

[1] U. Oberhagemann et al. , *Angew. Chem. Intern. Ed.,* **1996**, *35*, 2869.

**Keywords: layered, silicate, structure**

## MS68.P01

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**Large 2D-PSD for neutron single crystal structure analysis**

Yukio Noda,[a] Yoshihisa Ishikawa,[a] ChangHee Lee,[b] ShinAe Kim,[b] MyungKook Moon,[b] [a]*Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, (Japan).* [b]*HANARO, Korea Atomic Energy Research Institute (Korea).* E-mail: ynoda@tagen.tohoku.ac.jp

For structure analysis of complicated hydrogen-included materials, neutron single crystal structure analysis is very powerful tool. In addition, neutron single crystal experiment is indispensable for magnetic structure analysis for complicated magnetic system such like multiferroic materials. Usually, four-circle diffractometrs are used to accumulate intensity data. The only difficulty is the lack of efficiency of the measuring time due to the low flux of neutrons in general. Usually it requires long beam time, and sometimes, it is impossible to carryout. In order to overcome such low efficiency on single crystal neutron experiments, we have developed a large two dimensional position sensitive neutron counter (2D-PSD), and applied to structure analysis.

The large curved 2D-PSD for neutrons we have developed has an active area size 937 x 520 mm2. The radius of the detector is 535 mm, and the two-theta resolution is 0.2 degree /CH (Fig. 1). Two detectors were fabricated and installed at KAERI-HANARO and JAEA-JRR3. As the test experiment, standard samples NaCl and Tb3Fe5O12 (TbIG) are used. We could successfully performed structure analysis of TbIG with the following exposure conditions: the continuos rotation speed of the crystal is 0.4 degree/min, and 120 degree is covered, and exposure time is 5 hours. 962 Bragg points are covered including 181 absent Bragg reflections by symmetry. This is almost 10-20 times effective for consuming time compared with a conventional four-circle diffratometer. Not only the efficiency, we can survey unknown Bragg spots showing cell doubling at phase transition for instance. One of the 2D-PSD will be instilled at the dedicated beam port at HANARO.

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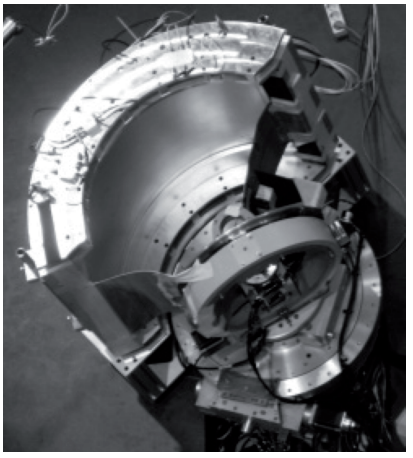

**Fig 1. 2D-PSD**

**Keywords: 2D-PSD, neutron diffraction, structure analysis**

## MS68.P02

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**Data correction of a novel CMOS detector**

Joerg Kaercher, Michael Ruf, Roger D. Durst, Greg Wachter, *Bruker AXS Inc., Madison, WI, (USA).* E-mail: joerg.kaercher@bruker-axs.com

Area detectors typically have systematic measurement errors that must be calibrated and corrected before the data can be used for crystallography. The techniques for the correction of CCD data are well established. However, the newest generation of CMOS based detectors presents new challenges. In particular, CMOS detectors exhibit low level nonlinearities and line-to-line offset noise (so called reset noise). This fixed pattern variation must be characterized and requires compensation. Here we describe the characteristics of CMOS detectors, the origin of these systematic errors and the techniques that can be used to correct them. The algorithms presented have been implemented in a special purpose processor for real time correction of the data stream from a CMOS detector. For this purpose the detector was equipped with considerable FPGA processing power. This is essential in order to dynamically normalize data at the pixel level for minor variations in intensity responsiveness.

**Keywords: detector, CMOS, software**