in the range between 15 and 250°C reveals the occurrence of at least two partially dehydrated phases. From the evaluation of the collected patterns it can be concluded that the principal crystallographic differences between these two materials and the kanemite structure are due to a pronounced decrease of the lattice parameter perpendicular to the silicate layers (direction [010]).

An ab-initio structure determination by simulated annealing of the first dehydration product of kanemite with nominal composition $NaSi_2O_4(OH)*H_2O$ was successful. Whereas the silicate layers of the kanemite structure are retained almost unmodified, pronounced changes can be observed in the interlayer sheet containing the Na cations. The previously unknown phase adopts space group *Pbcn* as well. Lattice parameters at ambient conditions are as follows: a=4.888, b=15.332, c=7.203Å.

[1] L.A.J. Garvie, B. Devouard, T.L. Groy, F. Camara, P. Buseck, *American Mineralogist* **1999**, *84*, 1170-1175. [2] S. Vortmann, J. Rius, B. Marler, H. Gies, *European Journal of Mineralogy* **1999**, *11*, 125-134.

Keywords: hydration, transition, silicate

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Data reduction of area detector measurements

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Time of flight Laue neutron diffraction a powerful tool to sample reciprocal space in a highly effective manner by collecting scattering data of a wide wavelength band simultaneously. Efficiency is further improved by highly pixelated large area detector coverage with excellent time resolution. This produces a wealth of data with every sample setting. Consequently large files of raw data need to be handled for data visualization, raw data corrections for incident spectrum variations, detector efficiency, background, sample effects and contributions. Furthermore, the software needs to be easy to use by new and experienced users alike. An increasingly important part of data collection is a strategy software that allows to tailor the measurement time and conditions to the sample symmetry and resolution requirements.

Examples of new and improved software developed and implemented at the TOPAZ single crystal diffractometer at the Oak Ridge National Laboratory will be presented. CrystalPlan helps define the measurement strategy and ISAW EV analyzes live neutron event data on the fly.

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Applications of area detectors to texture measurements

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The use of 2-dimensional detectors in Quantitative Texture Analysis (QTA) has been pointed out long ago mainly in order to reduce acquisition times, both at x-ray and neutron diffraction instruments [1], [2]. Indeed, the necessity to acquire several pole figures to correctly refine the orientation distribution functions makes indispensable their simultaneous acquisitions. Since typically 1000 pole figure points have to be measured, using point detectors creates very often acquisition times over several days, a dramatic drawback particularly at scarce neutron beam times. Historically, the development and use of linear, then curved position sensitive (CPS) detectors helped in reducing the acquisition to several hours [3], even at neutron steady state reactors [4]. Furthermore, it opened the way to the treatment of the whole pattern simultaneously including QTA information and more, a procedure nowadays called Combined Analysis [5]. CCD cameras and image plate systems further offer fast QTA analysis with no loss in the capability of full-profiling the patterns. Curvature of image plate detectors can be operated to create cylindrical solid angles for x-ray instruments, and at neutron lines, shaping parts of cylinders with individual detector plates or wires has been recently developed. For all these 2D-detectors, the aim to reduce the number of sample orientations to be measured has been at least partly achieved.

We will illustrate the main scheme used to construct pole figures and calculate ODFs from area patterns, giving some exemples of the use of Combined Analysis, which includes the determination of structure, phase and microstructure also. One of the last developments allowed by the use of Curved Area PSDs is the determination of Magnetic Quantitative Texture Analysis [6], which we will illustrate also.

[1] F. Heidelbach, C. Riekel, H.-R. Wenk *Journal of Applied Crystallography* **1999,** *32,* 841-849. [2] H.-R. Wenk, A.C. Larson, P.H. Vergamini, A.J. Schultz *Journal of Applied Physics* **1991,** *70,* 2035-2040. [3] J.-J. Heizmann, C. Laruelle, *Journal of Applied Crystallography* **1986,** *19,* 467-472. [4] H.-J. Bunge, H.R. Wenk, J. Pannetier *Textures and Microstructures* **1982,** *5,* 153-170. [5] D. Chateigner Ed.: **2010**, Wiley-ISTE, 496. [6] D. Chateigner, B. Ouladdiaf, F. Léon. *Solid State Phenomena* **2010,** *160,* 75-82.

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Modern trends in area detectors for single-crystal neutron diffraction

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Neutron single-crystal diffraction is the tool of choice to determine the accurate positions of hydrogen atoms in solids and the arrangements of magnetic moments. In some cases, hydrogen positions can be inferred from the positions of the other atoms, but if hydrogen bonding occurs, this is not reliable. Since neutron fluxes are typically low compared to those available at synchrotron X-ray facilities, there has been a major effort to maximize the exploitation of the available scattering data. Much emphasis has been placed in particular on the provision of large area detector systems. The D19 diffractometer at the ILL which has been equipped with a 120º x 32º multiwire proportional counter since 2007 provides greatly improved data quality for crystallographic work in structural chemistry, physics and the biosciences.

Another slightly less precise single-crystal diffraction method is the Laue method where the crystal is illuminated by a broad spectrum of wavelengths, and a large area of neutron-sensitive image plates (VIVALDI at the ILL, KOALA at ANSTO) is used to measure