smectites as a function of time, location and temperature. As the reusability of the moulding sand is critically related to the hydration and dehydration of smectite, we designed experiments to investigate of the dehydration kinetics in-situ. At the neutron radiography beamline ANTARES (FRM II, Germany) we simulated a casting process by dropping a special casting mould filled with moulding sand (12 wt% bentonite) on a hot copper plate (Figure 1). The design ensured an ideal heat transfer corresponding to the thermal shock-like heat induction during the real casting process. With this experimental set up, we were successful to in-situ visualize water fluxes within the moulding sand quantitatively with high temporal and spatial resolution. Thermocouples placed within the moulding sand simultaneously provided information on the temporal temperature gradients.
The experiments revealed a progressive movement of water in the sand and resolved a broad transitional zone from the pristine hydration state of the sand to a fully dehydrated state. At this transitional zone positions can be determined which on the one hand relate to the onset of pore water dehydration and on the other hand relate to the completion of interlayer dehydration. Thus, the experiments allowed us to successfully simulate the shock-heating of the mould material in a industrial casting process. The consequence of the shock-heating is a strongly non-linear temperature-time-position relation convoluted with the diffusion processes. A quantitative evaluation of the simulation data will be presented.

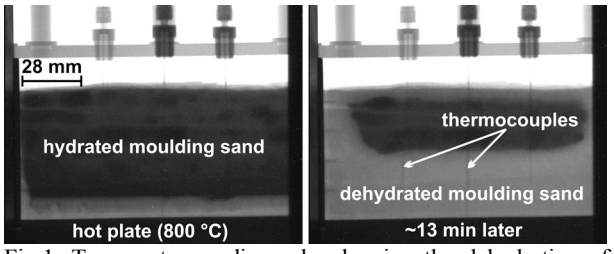

Fig.1. Two neutron radiographs showing the dehydration of the moulding sand. The process initiates at the hot bottom. The transitional zone between the pristine hydration state (top) and the fully dehydrated state (bottom) can be seen.

Keywords: smectites, interface processes, neutron radiography

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Surface and embedded 2-dim structures: a direct space approach to modelling.

Armin Kirfel[a], Karl F. Fischer[b], [a]*Steinmann Institute, University Bonn, Germany,* [b]*Technical Physics, University of Saarland, Germany*
E-mail: kirfel@uni-bonn.de

In the parameter space concept developed for the determination of 1-dimensional structures or structure projections without Fourier inversion, an arrangement of m equal scatterers is represented by a vector $\mathbf{t}(x_1, x_2, \ldots x_m)$ defined in space $\mathbf{P}^m$ [1,2]. Given a suitable number $n \geq m$ of observed intensities of reflections h, the principal objective of this approach is to find those test vectors $\mathbf{t}_t$ for which the best overall agreements between the observed $e(h)_{obs}$ and the model $e(h)_{calc}$ are obtained. The $e(h)$ are normalized structure amplitudes on absolute scale according to $e(h)^2 = n \cdot I(h)/\Sigma I(k)$, $k = 1,\ldots n$ [3], and the $\mathbf{t}_t$ proposed are fit to start a refinement procedure. Thus, it should be noted that (i) neither structure metrics nor any structure factor phases are needed, (ii) high spatial resolution is obtained from rather few experimental data, and (iii) homometric and quasi-homometric structures are automatically included. - The 1-dimensional approach was successfully tested in numerous examples with equal or nearly equal scatterers up to $m = 20$. In addition, we have shown that it is possible to reconstruct a 3-dimensional structure from the solutions obtained from up to 13 structure projections reflected in the central reciprocal lattice rows with low indices, *e.g.* $h00$, $0k0$, $00l$, $hh0$,…hhh *etc* [3]. - Encouraged by our experiences with the 1-dimensional structures we have started to apply the approach to simple acentric 2-dimensional structures or structure projections of symmetry ***p*1** with emphasis on exploring (a) the number(s) of scatterers m that can be handled in feasible PC computing times and (b) the numbers and kinds of reflections needed for finding test vectors $\mathbf{t}_t(x_1,y_1; \ldots x_m,y_m)$. - In ***p*1**, one scatterer (preferably the strongest) in (0,0) fixes the origin so that the problem is reduced to (m-1). In principle, there are two ways to generate $\mathbf{t}_t$'s, namely the systematic one by employing grid techniques (with the problem of finding the optimal spacing) and a random one (which is not necessarily inferior). Confining the discussion to the first technique we consider four basic strategies, *i.e.* the (i) exclusive use of a 2-dimensional grid and of general reflections hk, (ii) use of 1-dimensional x- or y-projection results based on reflections $h0$ or $0k$, respectively, with subsequent inspection of the corresponding rods at the proposed x_i or y_i to find the missing information from hk reflections, (iii) use of x- and y-projection results from $h0$ and $0k$ reflections, respectively, followed by finding correct (x,y) combinations from hk reflections, and finally, (iv) as (iii) but finding the correct (x,y) combinations with the aid of results obtained from reflections hh and $-h,h$, *i.e.* additional projections onto the directions [11] and [-1,1]. - Advantages and shortcomings of the different approaches with respect to structure sizes and computing times are compared, and including data errors examples of structure determinations are presented. Also addressed are possible extensions and applications, for instance in electron diffraction.

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Keywords: two-dimensional structures, phase problem eliminated, high resolution

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Dopant Effect on Surface Electronic State of TiO_2 estimated by First Principles Calculation.

Dong-Yoon Lee, Seung-Il Cha, Sun-Hee Seo, *Nanohybrid & Energy Materials Research Center, Korea Electrotechnology Research Institute, R. of Korea*
E-mail: dylee@keri.re.kr

The surface electronic states of TiO_2 doped with various metallic elements on Ti site were estimated by the discrete variation X_α (DV-X_α) method, which is a sort of the first-principles molecular orbital method and uses the Hatre-Fock-Slater approximation.[1] The energy levels, the partial density of state and the charge densities were calculated by using cluster models for bulk and surface.