organic crystals due to their softness causing them to crack.

Therefore we have developed and tested different methods to obtain the required quality and low roughness surfaces of soft organic crystals. All polishing methods are based on a high speed air bearing which can be equipped with different tools. The crystal is mounted on a piezo driven x-,y-,z- stage and can be moved with respect to the polishing device.

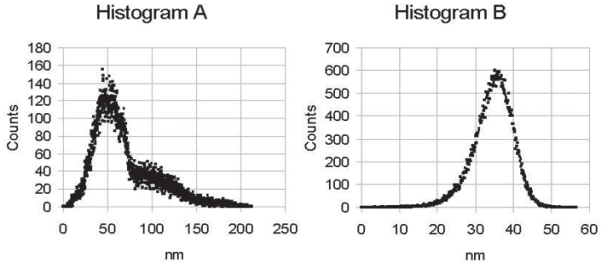
Beside different conventional polishing heads containing diamond grains of different sizes a custom made dimaond cutting tool was used. It consists of a monocrystalline diamond knife which is rotating perpendicular to the crystal surface.

The crystal surfaces generated with the different methods were characterized by atomic force microscopy (AFM). We used tapping mode imaging to reduce the forces on the crystal during the scanning process. The best quality surfaces possess a root-mean-square (rms) roughness of 5.3 nm for a 5 μm x 5 μm area. The rms roughness for a 80 μm x 80 μm area which corresponds to about 75 % of the whole crystal surface is about 14.8 nm.

We also cutted crystals using a commercial microtome suitable for electron microscopy sample preparation. Surfaces with a rms roughness of 4.7 nm for a 50 μm x 50 μm area and 2.9 nm for a 5 μm x 5 μm area could be achieved.

One big advantage of the air bearing cutting device compared to the microtome is the fast and easy processing of a large amount of crystals with high quality surfaces suitable for crystallographic and related experiments.

The figure below shows the histograms of height levels of a crystal polished by a conventional polishing head (A) and a crystal polished by the diamond knife tool (B).



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Keywords: organometallic, AFM

MS35.P38

Acta Cryst. (2011) A**67,** C469

Compositional distribution of isomorphic crystals during spontaneous crystallization

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A non-trivial bimodal distribution of crystals in the isomorphic composition was revealed at spontaneous mass precipitation in aqeuos solutions. Crystal ensembles of the series $(Pb,Ba)(NO_3)_2$, $(Co,Ni)(NH_4)_2(SO_4)\cdot 6H_2O$, $(Co,Ni)K_2(SO_4)\cdot 6H_2O$, $(NH_4,K)H_2PO_4$, $(Al,Cr)K(SO_4)_2\cdot 12H_2O$, and K(Cl,Br) were precipitated during 10–15 s in solutions of various isomorphic ratios at the supercoolings 10 °C and 20 °C. Precipitates were dried by filter paper after the solution decantation.

The isomorphic ratios in individuals of each the series were determined for random samplings of 100–120 individuals and some control samplings up to 400–500 crystals. X-ray fluorescence was used for $(Co,Ni)(NH_4)_2(SO_4)_2\cdot 6H_2O$ and $(Al,Cr)K(SO_4)_2\cdot 12H_2O$. Synchrotron-based XRF (ANKA FLT beamline, Karlsruhe) was used for the $(Pb,Ba)(NO_3)_2$ and $(Co,Ni)(NH_4)_2(SO_4)_2\cdot 6H_2O$ samplings [4]. Microprobe analyser ABT-55 Link AN 100000/85S was used for $(Co,Ni)(NH_4)_2(SO_4)_2\cdot 6H_2O$, $(Co,Ni)K_2(SO_4)_2\cdot 6H_2O$, and $(Al,Cr)K(SO_4)_2\cdot 12H_2O$ [4]. XRPD was used for the probes of K(Cl,Br), sieved to the fractions <10, 10–30, 30–50, 50–100 and >100 microns. Isomorphic compositions of crystal ensembles $(NH_4,K)H_2PO_4$ and K(Cl,Br) were also estimated by means of X-ray micro-tomography (SkyScan 1172).

The compositional distributions are asymmetric with two modes. However the bimodality is not quite clear sometimes due to such samplings were selected without the finest fractions. The distributions are sensitive to the probe total composition and supercooling: the peaks move regularly to one of the end-member. The XRD measurements for the series $(Pb,Ba)(NO_3)_2$ and K(Cl,Br) displayed a nonlinear function of the composition on crystals sizes [3]. The compositional bimodality is coordinated with that of the surface nuclei observed by AFM on a crystal surface of the mixed potassium-rubidium diphthalate [1]. This is in accordance with a high dispersion of crystal composition measured on a surface of grown $(Pb,Ba)(NO_3)_2$-crystals [5].

The compositional bimodality can be understood by the developed concept of mixed crystal formation [1, 2]. It establishes nucleation of two kinds caused by kinetic factor and displayed by modified concentration diagrams.

Results obtained by different analytical methods show that spontaneous mass crystallisation as well as monocrystal growth of solid solutions lead to formation of crystals with rather complex compositional distributions. These data confirm substantially the concept of mixed crystal formation [1].

Support by RFBR grants (10-05-00891, 10-02-01303) is gratefully acknowledged.

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Keywords: mass crystallization, isomorphism

MS35.P39

Acta Cryst. (2011) A**67,** C469-C470

A comparison towards counter-diffusion and sitting drop-vapor diffusion technique in improving resolution data of a novel organic solvent tolerant lipase

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Quality of diffraction data is important in order to generate a better electron density map which provides valuable, accurate information and enzyme functions in structure analysis afterward. To achieve the above objective, one way is to applied different kinds of crystallization techniques. In this study, we discussed about the improvement of crystal quality by counter-diffusion technique and sitting-drop-vapor diffusion technique.