

**P.16.01.1***Acta Cryst.* (2005). A61, C437**Use of reductive methylation of proteins to increase crystallization efficiency at the Midwest Center for Structural Genomics**Youngechang Kim, P. Quartey, L. Lezondra, C. Hatzos, M. Zhou, N. Maltseva, H. Li, R. Wu, A. Joachimiak, *Biosciences Division, Midwest Center for Structural Genomics and Structural Biology Center, Argonne National Laboratory, 9700 S. Cass Ave., Argonne Il 60439, USA*. E-mail: ykim@anl.gov

The highest attrition rate in high-throughput structural genomics (SG) projects utilizing x-ray crystallography occurs at the step of obtaining diffraction quality crystals. The Midwest Center for Structural Genomics (MCSG) has developed and continues to optimize the high-throughput crystallization pipeline. The pipeline was set up with nano-liter crystallization robots such as Honeybee and Mosquito, and a Matrix Maker equipped with Crystal Monitor software for screening initial crystallization conditions and crystal optimization. As a part of effort to increase the success rate of obtaining diffraction quality crystals, chemical modification of proteins has been tested in the MCSG crystallization pipeline. Particularly, reductive methylation of lysine residues to alter the crystallization properties has been evaluated with more than 100 proteins, most of which have not been crystallized previously. Following the method described by Ivan Rayment (in Volume 276 of *Methods of Enzymology*) the proteins were methylated and screened using standard MCSG crystallization pipeline. Several structures have been obtained using this approach and detailed analysis and progress will be presented.

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**Keywords:** reductive methylation, structural genomics, attrition rate

**P.16.02.1***Acta Cryst.* (2005). A61, C437**Implementation of a Novel Protein Crystal Image Analysis Package**Daniel C. Frankel<sup>a</sup>, Rhett Affleck<sup>b</sup>, <sup>a</sup>*Bruker AXS, Madison Wisconsin*. <sup>b</sup>*Discovery Partners International, San Diego, California*. E-mail: dan.frankel@bruker-axs.com

Crystal Resolve is automated image analysis software for protein crystallography. It is offered as an add on package for the Crystal Farm product line.

Crystal Resolve uses proprietary high precision subpixel image processing and object recognition algorithms to decompose an image into thousands of significant micro features. It applies specific knowledge of the drop type and plate geometry along with neural networks and advanced heuristic methods to classify these features while developing a macroscopic comprehension of image contents. From this, it computes two key metrics.  $F_C$  describes how crystal-like (0.0-1.0) the image is.  $F_P$  describes how precipitate-like the image is.

For all its complexity, Crystal Resolve is very easy to use. Users are given the flexibility to choose which images should be reviewed in terms of their  $F_C$  and  $F_P$  values. Crystal Resolve easily identifies images with no interesting content, greatly saving researchers' time.

Crystal Resolve benefits projects with hard to find crystals by allowing users to select and view images with poorer  $F_C$  figures. Crystal Resolve frequently finds objects that some crystallographers miss while not getting confused by dust, bubbles, and plate features.

Some examples of analyzed images from different crystallization plates will be presented.

**Keywords:** protein crystallization, imaging, protein crystal growth

**P.16.03.1***Acta Cryst.* (2005). A61, C437**AFM Observation and Morphing-reconstruction of Dynamics of Crystal Growth**Natalya N. Piskunova, *Institute of Geology of Komi Science Centre of**Ural Branch of the Russian Academy of Sciences, Syktyvkar, Komi Republic, Russia*. E-mail: piskunova@geo.komisc.ru

With *in situ* investigations by an atomic force method (AFM) and using statistical approach we studied evolution of the crystal surface of sodium chloride in the solution. The determined mean values of tangential rate and distances between the steps for every interval showing a normal rate of the growth of the scanning area associating with thermodynamic conditions of growth [1]. Tangential rate of movement of each step is calculated by comparison of two successive snapshots. But not always the following AFM snapshot can be wrong for such comparison with the previous. Or statistics requires recovering a picture of the surface at the "offscreen" interval between two snapshots that is 40 sec. In crystallogenic investigations there is often necessity for dynamic reconstruction of the occurring processes. Currently, there is a number of graphic programs as morphing programs enabling to estimate up to 100 intermediate images and thus, to obtain an image of a surface each 0.4 sec and to use the estimated images for statistical calculation. Moreover, it is important that all images can be combined as motions. We have made several demo videotapes with duration of 1 to 6 minutes used at the lectures for university students as visual aids showing peculiarities of development of the surface structure, formation of solution inclusions, surface growth in the directed flow of the solution.

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[1] Piskunova N.N., Rakin V.I., *Proceedings of ICCG-14*, Grenoble, 2004, 347.

**Keywords:** AFM, crystal growth from solution, surface morphology

**P.16.03.2***Acta Cryst.* (2005). A61, C437**Catalysed Growth of Doped TGS Single Crystals with Pt(IV) Ions**Jan Novotný, *Institute of Radio Engineering and Electronics, Academy of Sciences of the Czech Republic*. E-mail: novotny@ure.cas.cz

The exploitation of the ferroelectric triglycine sulfate,  $(\text{NH}_2\text{CH}_2\text{COOH})_3\cdot\text{H}_2\text{SO}_4$  (TGS) in some technical applications [1] has increased the need for high-quality single crystals with stabilized domain structure [2].

A novel type of full faceted single crystals of triglycine sulfate with various contents of Pt(IV) complex-forming ions and L-alanine, D-phenylalanine or L-arginine were grown from aqueous solutions. Morphology, domain structure and *P-E* hysteresis loops have been investigated.

On the wafers prepared from  $\langle 110 \rangle$  pyramids we measured the main physical properties, in particular: spontaneous polarization  $P_s$ , coercive field  $E_c$ , internal electrical field  $E_b$ , dielectric permittivity  $\epsilon_r$ , and dielectric losses  $\tan\delta$ .

The effect of the dopant on the growth velocity is explained on the basis of catalytic action of supposed platinum complexes [3]. The value of  $E_b$ , important for technical applications of grown crystals, can be adjusted by Pt(IV)-ions concentration in the growth solution.

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[1] Whatmore R.W., *Rep. Prog. Phys.*, 1986, **49**, 1335. [2] Neumann N., *Ferroelectrics*, 1993, **142**, 83. [3] Novotný J., Březina B., Zelinka J., *Cryst. Res. Technol.*, 2004, **39**, 1089.

**Keywords:** crystal growth, ferroelectric crystals, domains

**P.16.03.3***Acta Cryst.* (2005). A61, C437-C438**Crystallization of Water-soluble Inorganic Salts in Microwave Field**Sergey E. Kochetkov<sup>a</sup>, Viktor A. Kuznetsov<sup>a</sup>, Alexandr V. Ljashenko<sup>b</sup>, Vyacheslav S. Bakshutov<sup>b</sup>, <sup>a</sup>*Institute of Crystallography*