MS12-O2 Protein crystal transformation – new insights by new techniques

Reiner A. Kiefersauer[1,2], Breyan H. Ross[1,2,3], Robert Huber[1,3,4,5]

1. Max-Planck-Institut für Biochemie, Am Klopferspitz 18, 82152 Martinsried, Germany
2. Proteros Biostructures GmbH, Bunsenstrasse 7a, 82152 Martinsried, Germany
3. Technische Universität München, Lichtenbergstrasse 4, 85747 Garching, Germany
4. Zentrum für Medizinische Biotechnologie, Universität Duisburg-Essen, 45117 Essen, Germany
5. School of Biosciences, Cardiff University, Cardiff CF10 3US, Wales

email: kiefersauer@proteros.de

Protein crystallography is the main technique to obtain structural information of biomolecules at atomic level, but requires crystals of sufficient quality and order. We designed and constantly developed a technical platform for post-growth crystal treatment based on a freely mounted crystal stabilized by a humidified gas stream combined with optical dimensional control of the crystal and analysis of its quality by X-rays ([1,2]Free Mounting System).

In the presentation we will briefly introduce in this technique and describe the control of the crystal system during the process. Starting from the native crystal, disorder can be clearly addressed in the whole process (native crystal quality, crystal treatment, and freezing) and subsequently modulated and improved.

The addition of chemicals to the crystal by the deposition of small droplets (~ 30 picoliter) directly onto the crystal surface (Pico dropper) allows the systematic study of the influence of compounds as e.g. glycerol, polyethylene glycol, [3]trimethylamine N-oxide, heavy metals to the crystal order. The increase of compound concentration in fine steps controlled by measuring the crystal extension and crystal order simultaneously allows to find the optimal concentration. After crystal treatment, the crystal can be readily frozen within a second by a mechanical switch from the humid gas stream to the cold gas stream for data collection.

We discovered that heating of the protein crystal by IR-Laser irradiation continuously or in pulses has the potential of inducing new physical [2]processes. The speed of crystal shrinkage driven by light can play an important role in improving crystal order. Variation in the experimental setup (crystal in the cold gas stream, crystal under oil) combined with heat application offers new strategies for crystal annealing and improvement.

Overall, understanding of crystal transformation is a pre-condition for the evaluation of ideas about crystal optimization. Examples of crystal transformation on a macroscopic and microscopic scale will be shown in this presentation ending in an outlook for future work.

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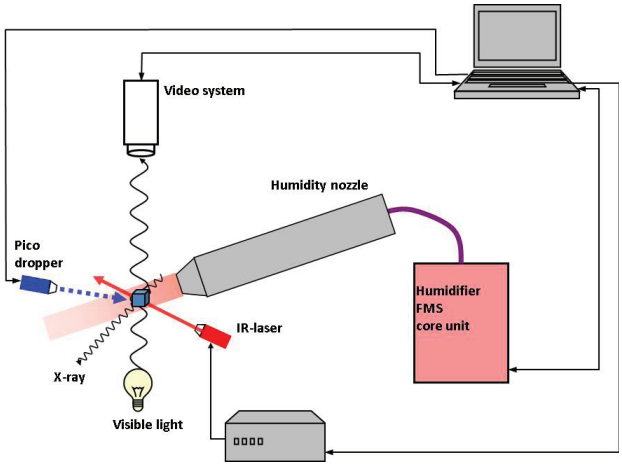

Figure 1. The protein crystal is held in the humidified gas stream and analyzed by X-rays (microscopic effects) and by a video system (macroscopic effects). The crystal is treated by heat (IR-laser) or / and by droplets of solution (Pico dropper). Optional combination of hardware for automation is possible.

Keywords: protein crystal, crystal transformation, dehydration, IR-laser, crystal improvement, crystal annealing