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Report:

The photosystem I (PSI) from the cyanobacterium *Synechococcus elongatus* serve as model to elucidate the influence of microgravity on crystal growth and the quality of the crystals. The crystallisation of the large membrane protein PS I was achieved under microgravity on the STS-95 mission. During this beamtime crystals grown during the STS-95 mission have been investigated. Comparison of the microgravity to the ground control experiments shows a significant influence of the microgravity on the nucleation rate, crystal growth and mosaicity. These results could led to a better understanding of the nucleation rate and crystal growth. It could be from special interest, that the nucleation process over a fluid crystalline phase, in which crystals order in 2-dimensional detergent layers.

Ten partial data sets of native PSI crystals grown under microgravity and two data sets of corresponding ground control were collected. Each data set was obtained by a total rotation of at least 16° about the spindle axis of the goniometer. In order to get a better statistics small crystals were grown during this mission with dimensions of 0.1 mm in diameter and 0.5 mm in length. All space grown crystals diffracted from 3.0 Å to 3.3 Å. The diffraction was

mainly limited by the small size of the crystals. The mosaicity was in the range of 0.5°. Corresponding crystals grown under normal gravity had dimensions of 0.3 mm in diameter and 0.5-1 mm in length, but they diffracted only from 4.0 Å to 8.0 Å. The mosaicity was in the range of 0.8° to 5°. The evaluation of these data is in progress.
Partial diffraction data sets collected from native PSI crystals grown under microgravity conditions are superior in diffraction quality to those of ground. These crystals diffract to higher resolution with lower mosaicity, possibly demonstrating the usefulness of microgravity in the crystallisation of proteins especially of membrane proteins. It would be very interesting to crystallise photosystem I under microgravity using seeding techniques in the future, which have led on earth to the recent improvement of the crystals 2.5 Å (Jordan et al., 2001)

Ferredoxin from the thermophilic cyanobacterium *Synechococcus elongatus* is an electron carrier between PSI and ferredoxin-$NADP^+$-reductase. Electrons are transferred from PSI to a soluble ferredoxin containing anFe_2S_2 cluster and located in the stroma. Reduced ferredoxin reduces $NADP^+$ in a reaction driven by the ferredoxin-$NADP^+$-reductase.

We collected data form different PSI/ferredoxin complexes, using different crystallisation techniques and conditions for growth of the PSI/ferredoxin crystals. These data sets are of comparable quality as the data set collected during the beamtime allocation time LS-1503. The question whether these crystal belong two the space group $P2_12_12_1$ nor to $P22_12_1$, which is important for the structure determination, is still under investigation.

We also collected a data set of photosystem II cocrystallised with the herbizide Karbutylat. Three month ago during the beamtime allocation time (LS-1802) we had already collected a data set with the herbizide Ioxynil.
We collected from crystal a data set to ~ 3.9 Å resolution with a completeness of 97.9 %. The data were processed with DENZO and SCALEPACK and led to the following statistics: Rsym=0.09 and $<I/\sigma(I)>=8.0$ (Rsym=0.4 $<I/\sigma(I)>=2.2$).
In the difference electron density map, we identified additional density. In the surrounding of the binding pocket we observed deformation in the protein backbone. Further data sets at higher resolution have to be collected to allow a detailed prediction of the amino acids involved in herbicide binding.

Reference

Jordan, P., Fromme, P., Witt, H.-T., Klukas, O., Krauß, N., Saenger, W., (2001) Three-dimensional structure of cyanobacterial photosystem I at 2.5 Å resolution. *Nature* **411**, 909-917.