(200) and (020) reflextion can not be measured separable and are consider as one line. The second one CPO index [0 10 0]/[10 0 10] distinguish between (100) and (010) orientation. Because of overlapping with several others diffraction the second one index can be used only when the first one is close to one, in this case the intensity of (0 10 0) and (10 0 0) diffraction are much more bigger than the other reflection diffracting to this area.

Conclusions

The CPO indexes given by X-ray diffraction compared with SEM micrograph helps in understanding the grooving of MFI thin layers and their preferred orientation on the surface of studied supports.

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Table 1. CPO indexes for several samples

Sample	CPO	
	[200+020]/[133]	[0 10 0]/[10 0 0]
17-08 (floating)	0.99	0.33
3z - 08	0.84	0.68
16-08	-18	0.70

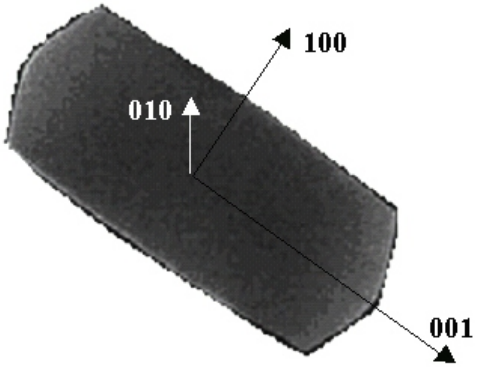

Figure 4. The relation between macroscopic grain shape and crystallographic directions.

Tuesday, June 15, section A

SL6

CAN TRYPTOPHAN ENHANCE PROTEIN CRYSTALLIZABILITY?

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X-ray crystallography is a powerful tool in protein tertiary structure determination. For this method the preparation of well-diffracting crystals is inevitable, which usually represents the most problematic and rate-limiting step. The process of protein crystallization is influenced by many parameters and protein itself, its purity, homogeneity and properties, namely the ability of forming crystals, is the most important one. Many attempts were done with the aim to improve protein crystallizability and crystal quality. Protein modifications oriented on improvement in protein homogeneity, solubility, stability and/or crystal quality represent fruitful approach to solving the problem of high-quality crystals preparation. Besides chemical modifications of proteins, their truncations, deglycosylation, limited proteolysis, the mutations of individual amino-acid residues become very popular. A lot of examples of successful mutations can be found in the literature, however, no universal recipe exists and/or no absolute rules can be extracted. Hence the main question - which to which amino-acid should be mutated - is still valid.

Analysis of intermolecular contacts in the crystals of several different proteins crystallized in our laboratory revealed that tryptophans located at the molecular surface can form a number of intermolecular contacts in the crystals. The large size and the mixed hydrophobic/hydrophilic character of tryptophan side chain allow various kinds of interactions with a number of residues simultaneously. Tryptophans are usually mostly buried in the molecules, rather rarely they are exposed to the solvent. It is known that tryptophan residues have an important role in stabilizing the protein structures. Recently it has been observed that tryptophans located on the molecular surface can indicate the binding site.

These facts together with the above mentioned observations inspired us to analyze the role of tryptophan in formation the intermolecular contacts in crystals. For this, the systematic analysis of protein X-ray structures deposited in

PDB was performed. Structural data set of protein structures (resolution 1.2 Å or better) was prepared and analyzed on the presence of tryptophan residues and their location. It is known, that tryptophan is most rare amino-acid in protein structures therefore it was not surprising that up to 25 % of protein structures from the set did not contain any tryptophan. The atoms of indole ring of about 20 % of analyzed tryptophans were completely buried. On the other side, the indole ring of 12 % of tryptophans was classified as "fully exposed" to the solvent. Further inspection of these "fully exposed" tryptophans and crystal contacts mediated by their indole ring atoms led us to the conclusion, that tryptophan can be useful in protein crystallization. In spite of the possible negative influence of tryptophans with solvent accessible side chains on protein solubility, and maybe also other protein properties, we believe that tryptophans located on the protein surface might improve crystallizability of proteins and optimize crystal packing.

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SL7

BIOCHEMICAL AND STRUCTURAL CHARACTERIZATION OF NEW HALOALKANE DEHALOGENASE DBEA FROM *Bradyrhizobium elkani* USDA94

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A novel enzyme belonging to the family of haloalkane dehalogenases (EC 3.8.1.5) was isolated from *Bradyrhizobium elkani* USDA94. Haloalkane dehalogenases are important class of microbial enzymes with catalytic activity for detoxification of halogenated aliphatic compounds. DbeA protein is closely related to DbjA enzyme from *Bradyrhizobium japonicum* USDA110 (71% identity), but has different biochemical properties. DbeA is generally less active than DbjA and has a higher specificity towards brominated and iodinated compounds. Crystal structure of novel haloalkane dehalogenase DbeA of *Bradyrhizobium elkani* USDA94 has been solved and refined using diffraction data to 2.2 Å resolution. Overall fold and topology of DbeA is very similar to related enzymes with known structure. Structural comparison discovered differences in active site tunnel, which can explain differential substrate specificities and inhibitor affinities.

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SL8

CRYSTALLIZATION OF HIGHER PLANT PHOTOSYSTEM II

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The aim of this work carried out in collaboration with Laboratorio de Estudios Cristalográficos, (Granada, Spain) is to crystallize higher plant photosystem II (PS II) for high resolution X-ray diffraction study and resolve the structure of mentioned protein supercomplex.

The combination of centrifugation (sucrose density) and chromatography techniques (ion exchange, gel filtration) for extraction and purification of the PSII complex from solubilized thylakoid membranes of the *Pisum sativum L*. chloroplasts are used. The complex activity throughout the isolation routine with optical spectroscopy and polarographic measurements of oxygen evolution rates are tested. All possible methods and approaches for crystallization of both membrane and soluble proteins will be used to produce crystals of PSII in diffraction quality.

New protocol for hydroponics plant growth under controlled conditions has been already established. Nowadays the protocol for isolation of the PS II enriched thylakoid membranes is re-designed and implemented into testing. The screening for most suitable buffers and detergents that will sustain maximum PSII activity throughout the isolation routine will be performed. Later the crystallization trials of the PSII protein complex will be setting up.

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