ESRF	**Experiment title:** **S-layer protein of *Bacillus sphaericus***	**Experiment number**: **30.01.507**
Beamline:	**Date of experiment**: from: to:	**Date of report**: 18-10-2002
Shifts: 2	**Local contact(s)**: L. Jacquamet	*Received at ESRF:*

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Report:

The outer surface of the cells of some Bacteria and some Archaea is covered by single layers of protein subunits (S-layer) directly exposed to the environment. These subunits form primitive cell envelopes and may represent the most primitive biological membranes. They are involved in shape maintenance and in interactions with the environment. The S-layer represents the outermost cell envelope directly exposed to the often extreme conditions of their surroundings. The structure of a S-layer protein would help understanding the strategies developed by nature to survive in such conditions.

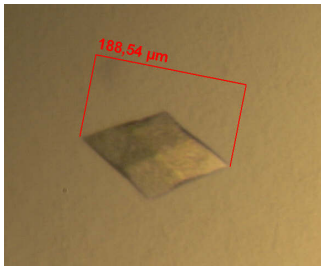

Fig. 1

The best crystals (Fig. 1) were grown with ammonium sulfate as precipitant, bicine pH 7.6 as buffer, in presence of the detergent n-Dodecyl-β-D-maltoside. The morphology of the crystals suggested the presence of a 4-fold axis, in good agreement with the results of electron microscopy (Fig. 2).

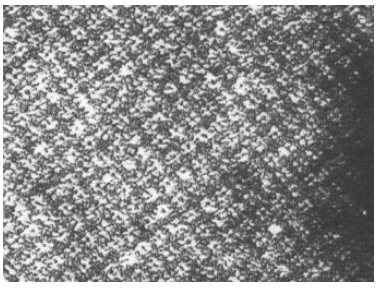

Fig. 2

Before data collection, the crystal was cryo-soaked for 45sec in the presence of 20% ethylene-glycol and 1.0M sodium bromide and MAD data were collected on beam line BM30A using the bromide ions as

anomalous scatterers. The crystals are tetragonal, space group I422, with a = 116.7 Å and c= 182.4 Å. The processing was performed with Denzo and Scalepack.

Data set	Peak	Inflexion	Remote high energy	Remote low energy
Wavelength (Å)	0.920257	0.920479	0.918417	0.979792
Resolution (Å)	3.7	3.7	3.7	3.7
Reflections				
total	50,903	27,192	21,726	24,749
unique	10,998	10,859	9,664	11,289
Completeness (%)	84.2	82.5	73.1	85.2
R_{merge}	0.150	0.109	0.136	0.091

In spite of the nice shape and the good dimensions of the crystal, the data are extremely weak. Up to now, intensive applications of the programmes "Shake and Bake" and SHELXD did not allow to determine the positions of the bromine atoms.