EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

Experiment Report Form

	Experiment title: Investigation of the crystallization process of proline on the (100)-surface of fluorapatite using GIXRD experiments and truncation rod crystallograph	**Experiment number**: CH-4307
Beamline: BM-25	**Date of experiment**: from: 29.04.2015 to: 05.05.2015	**Date of report**: 18.05.2015
Shifts: 18	**Local contact(s)**: María Vila Santos, Juan Rubio Zuazo	*Received at ESRF:*

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Report:

The measurement of CTRs will permit to determine the active sites of adsorption of the organic molecules on the fluorapatite surface and yield detailed information about the 3-dimensional structure of the interface between the mineral and a sorbate layer of proline molecules which act as nucleation seed for crystallization. When an ordered proline monolayer is formed, the orientation and position of the zwitterions can be compared with the binding sites and the adsorption mode of proline on the (100) surface (mono- or bidentate binding).

We were able to measure three datasets of CTRs and L-Scans, representing the fluorapatite (100) surface under different conditions, one with D-proline/D_2O, one with D-proline/H_2O and one with L-proline/H_2O solution on top of the surface. The first dataset of (100) fluorapatite with D-Proline/D_2O contains 14 nonequivalent CTRs and 19 reference scans in

anti bragg position as well as 10 L-Scans with CTRs for verification of the alignment. Also, four equivalent CTRs could be measured for comparison. The second dataset of fluorapatite (100) with D-proline/H_2O solution consists of 13 nonequivalent CTRs, 11 reference scans and 12 L-Scans with rocking curves for verification of the alignment. Because the measurements of the CTRs were very time consuming, 24 L-scans and only 12 CTRs were performed for the last data set.

From these extensive datasets, it will be possible to determine the (100) surface structure in contact with highly concentrated D-proline/D_2O-, D-proline/H_2O- and L-proline/H_2O solutions. It will be feasable to explore the proline-fluorapatite interface order with structural information on the adsorption site of the different proline molecules onto the surface as well as its molecular conformation and orientation. Thereby we can determine potential distinctions in the adsorption behavior of the differing solutions. Further the evolution with time of the proline/FAp interface structure (nucleation/degradation) can be followed by the measurement of the intensity dependence of the reference reflections in anti-Bragg conditions during the experiment. The effect of the different solutions on the experimental structure factors becomes obvious in the following figure, where the comparison of an exemplary CTR (3, 0, L) already shows slight differences in the intensities between the measurements of the liquid/solid interface structure factors after preliminary refinements.