CNR Short Term Mobility Program 2017

Il Fruitore: BUJAR DIDA

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Periodo: 22 Gennaio – 2 Febbraio 2018

Titolo del programma: Sviluppo routine in MATLAB per analizzare dati SWAXS nella modalità scansione per lo studio dei nano/biomateriali

Scientific Report

The activities performed during the two weeks (10 working days) visit at the Institute of Crystallography by Bujar Dida under supervision of Dritan Siliqi was focused at:

I. Developing routines to analyze Small/Wide Angles X-ray scattering (SWAXS) on scanning methods

X-ray scattering techniques such as small- and wide-angle X-ray scattering (SAXS and WAXS) are nondestructive approaches, widely applied to the study of, respectively, above- and sub-molecular structure ordering of materials or tissues, among other applications. The electron density inhomogeneity of the sample is monitored at the nanometre scale in SAXS (Craievich, 2005) and at the atomic scale in WAXS (Dorfs et al., 2011). The structural or morphological information can be inspected by working in transmission geometry (SAXS/WAXS) for thin samples or in reflection geometry (grazing-incidence SAXS/WAXS or GISAXS/GIWAXS) for materials deposited on top of surfaces or just underneath them (thin films, coatings, planar devices). In this latter geometry, the incidence angle is tuned on purpose across the surface total reflection angle to change the penetration depth of the X-ray beam below the surface accordingly (Renaud et al., 2009). Recently,

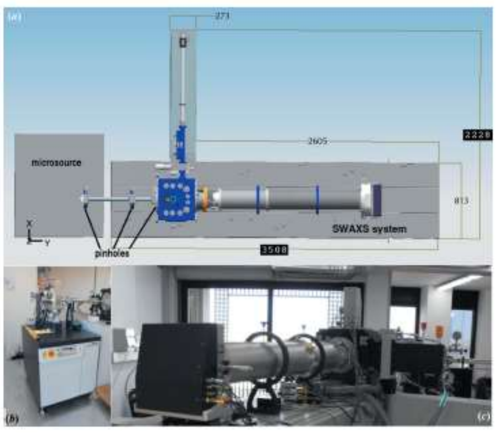

Figure 1
(a) Scheme of the XMI-LAB; (b) Fr-E+ SuperBright microsource; (c) SAXS/WAXS (SWAXS) three-pinhole camera.

SAXS/ WAXS scanning microscopy has been developed as an additional tool to investigate tissues or materials science samples through a focused X-ray beam, which is used to scan a specimen faster while acquiring SAXS and/or WAXS scattering patterns with a fast two-dimensional detector (Paris, 2008; Dunlop & Fratzl, 2010). SAXS/WAXS scanning transmission microscopy experiments are typically performed with synchrotron radiation (see e.g. Deyhle et al., 2011; Hexemer et al., 2010; Riekel et al., 2010). In our case the data were collected at IC-CNR XMIL@B using the instrumentation Rigaku SMAX-300 [Fr-E+ SuperBright Rigaku rotating anode copper anode microsource, Cu Kα, l=0.15405 nm coupled by means of a multilayer focusing optics (CMF 15-105) to a three pinholes camera] (Altamura et al, 2012) shown in Figure 1, and the data were analyzed by using SUNBIM package (Siliqi et al., 2016).

In Figure 2 is shown the flowchart used into SUNBIM. Our work was focused in following steps using MATLAB language:

a) Each twodimensional frame of the mesh is folded into a one-dimensional profile;

b) Two a more profiles (1D images) was selected as most representatives (typically, one as a background and two as signals) by adaptive binning approach (Ladisa et al. 2007);

c) Selection a region (in q range), corresponding to one or more diffraction picks. The length scales identify one or more tissue/material components (Figure 3a);

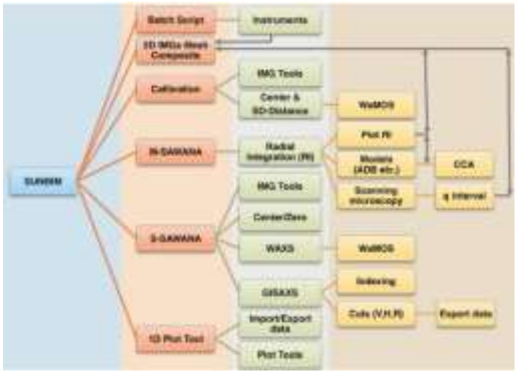

Figure 2. SUNBIM flowchart

d) According to the multi-modal imaging procedure, the intensity distribution along the azimuth of the selected rings is analyzed for each two-dimensional frame and transformed into microscopy images. For each monitored peak, the subtracted background can be evaluated by polynomial interpolation. Alternatively, an experimental background image can be subtracted from all the frames of the mesh.

e) The microscopy images, for a glance interpretation of the data, encode the local presence (color) or absence (black) of a specific tissue component, the orientation of a specific direction (color wheel) in the tissue (e.g. fiber orientation of collagen), and the degree of orientation (Figure 3b)

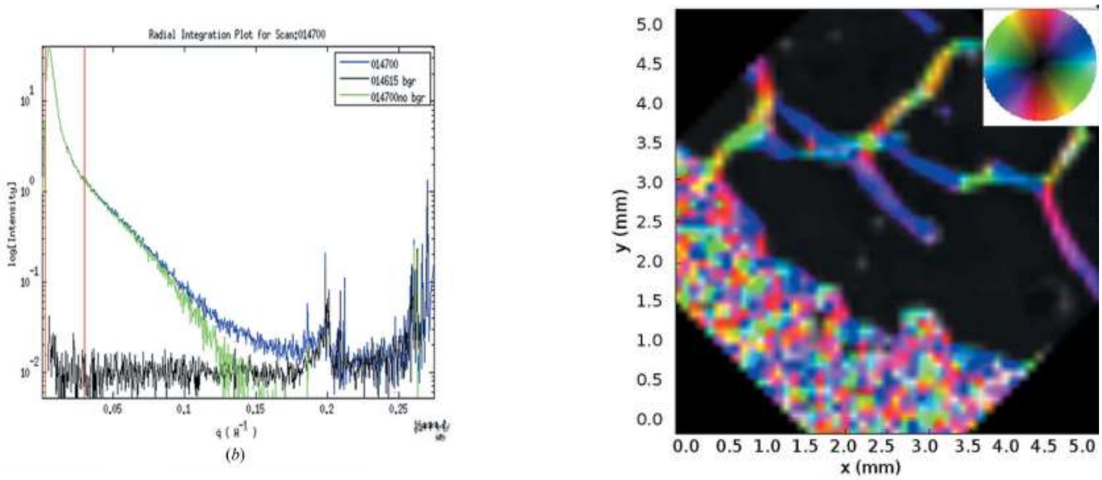

Figure 3. Scanning procedure example. (a) Radial integration and background subtraction example for one of the selected scans; (b) orientation map (color wheel indicates the direction);

II. This short term mobility was used even to prepare the further collaboration between FMIF, Tirana, Albanian with IC-CNR, Bari, Italy concerning new nanomaterials for applications in conservation and consolidation of stony materials part of Culture Heritage in Albania. In collaboration with the technician of **Bio-crystallization Lab** it was made a piloting tests of preparation on nanomaterials (NPs) of Sr(OH2) proving in that way a guidelines for the laboratory preparation (FIMIF,PUT in Albania) by identification of the best conditions and procedures.

III. Training on using XRD diffractometers (single crystal and powder diffraction) at IC-CNR laboratories and using the dedicated software (developed by IC-CNR, Bari), like SIR, SIRPOW, QUALX and SUNBIM.

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