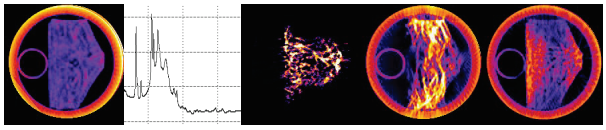
Keywords: X-ray diffraction analysis programming, KOSSEL diffraction, XRT technique

FA5-MS40-P07

Pressure anisotropy on C60-graphite transformation seen by diffraction-tomography. Jean-Louis Hodeau [a], Michelle Alvarez-Murga[b,a], Pierre Bleuet[c], Mohamed Mezouar[b], Remi Tucoulou[b], Christophe Lepoittevin[a], Nathalie Boudet[a], Jean-François Berar[a], Leonel Marques[d], [a]*Institut Néel, CNRS-UJF, 38042 Grenoble, France,* [b]*ESRF, BP 220, 38043 Grenoble, France,* [b]*CEA /LCPO & CEA-LETI, Grenoble 38054, France.* [b]*Univ Aveiro, Dept Fis, Ciceco, P3800 Aveiro, Portugal*
E-mail: hodeau@grenoble.cnrs.fr

The advent of heterogeneous and textured material calls for development of local structural probes to characterize them. The anisotropy of local heterogeneities, crystalline orientations and hierarchical architectures influences their macroscopic physical properties. This feature arises from the processing and thermo-mechanical history of the material and exists in natural and synthetic multiphase materials as diverse as biological tissues (bone, tooth), cements, nano-materials, alloys, pigments, mineral products or materials synthesized at high-pressures like carbon 3D zeolites [1].
Here we show the potential of "diffraction tomography" (XRD-CT) to study both phase and crystalline orientation distributions. This method has been recently demonstrated on multiphase materials provided some conditions are fulfilled [2]. Presently, the demonstration is performed on a textured heterogeneous C60polymer-graphite pellet obtained by high-pressure (5 GPa, 1100K) treatment using a Paris-Edinburgh cell setup [3]. In-situ XRD synthesis-measurements were done at beamline ID27 and "diffraction-tomography" experiments were performed at beamlines ID22 and BM02 at the ESRF. The spatial resolution of the probe has been tailored to be compatible with the grain size of the crystallized material, and beam sizes were 2×1 μm^2 and 100x100 μm^2 using 18 keV energy. Our results present both sample and texture orientation relationships as a function of the pressure direction.



Furthermore "diffraction-tomography" allows the extraction of known and unknown scattering patterns of amorphous and crystalline compounds with similar atomic densities and compositions. It can be carried out simultaneously with X-ray fluorescence, Compton, and absorption tomographies, allowing a *multi-modal* analysis of prime importance in materials science, geology, paleontology, cultural heritage and medical science, textured materials. textured materials.

[1] L. Marques et al. Debye–Scherrer ellipses 3D fullerene polymers: An anisotropic pressure memory signature. *Science* 1999, 283, 1720.
[2] P. Bleuet, E. Welcomme, E. Dooryhée, J. Susini, J.L. Hodeau, P. Walter, Probing the structure of heterogeneous diluted materials by diffraction tomography, *Nature Materials* 2008, 7, 468.
[3] G. Morard et al. Optimization of Paris–Edinburgh press cell for in situ monochromatic X-ray diffraction and X-ray absorption, *High Press. Res. 2007,* 27 , 223.

Keywords: diffraction-tomography, texture, fullerenes

FA5-MS40-P08

Conditions for reception of x-ray monochromatic bunches of the maximum intensity in geometry Laue. V.V. Margaryan, K.T. Hayrapetyan, S.N.Noreyan, *X-Ray Pungs Laboratory. Yerevan, Republic of Armenia*
E-mail: x-ray@web.am

In the presented work dependence of absolute value of intensity of monochromatic x-ray radiation, diffracted from a direction of a incidence primary bunch in a reflection direction in geometry Laue in the presence of external influences (a condition of a full pumping), from a thickness of a single-crystal is investigated. As is known, the angular width of a full pumping x-ray bunch, in the presence of external influences, depends as on a thickness of a single-crystal (t) [1], and from distance a radiation source - a sample [2]. At the fixed distance a radiation source - a single-crystal in process of increase in a thickness of a single-crystal the angular width of a full pumping x-ray bunch linearly increases.
From the previously mentioned follows, that with increase in a thickness of a single-crystal the sizes of angular area of a full pumping from a direction of a primary bunch in a reflection direction increase, integrated intensity of the reflected bunch therefore increases.
On the other hand, the increase in a thickness of a single-crystal leads to increase in the integrated intensity absorbed by a single-crystal. It is natural to assume, that in the described conditions, changing a thickness of a disseminating single-crystal, it is possible to find that optimum thickness at which the absolute value of a full pumping x-ray bunch in a direction of reflection will be maximum.
As a result of the detailed analysis of results of an experimental research it is shown, that the absolute size of integrated intensity full pumping from a primary direction in a direction of reflection of a x-ray bunch reaches the maximum at condition observance: $\mu t=1$, where μ - factor of linear absorption, t - a thickness of a single-crystal.
The validity of the given condition is confirmed also by theoretical calculations.

[1].С.Н. Нореян, В.К. Мирзоян, В.Р. Кочарян., Зависимость угловой апертуры полного перебрасываемого рентгеновского излучения от толщины монокристалла при наличии температурного градиента. Известия НАН Армения, Физика, 2004, Т.39, N2, С.124-130. [2].V.V. Margaryan, K.T. Hayrapetyan, S.N. Noreyan, The Peculiarities of Angular Width of Diffracted X-Rays at The Presence of Temperature Gradient, Acta Cryst. 2009. A65, s214

Keywords: X-ray diffraction, X-ray absorption, X-ray single-crystal diffraction

FA5-MS40-P09

Probing inclusions in diamonds with fine beams of synchrotron X rays Moreton Moore[a], Rais Shaikhaidarov[a], Victor Petrashov[a], Fanus Viljoen[b], [a]*Physics Dept, Royal Holloway University of London, UK,* [b]*Geology Dept, University of Johannesburg, South Africa*
E-mail: m.moore@rhul.ac.uk

Station B16 at the Diamond Light Source is a versatile test facility for trying out new experiments with synchrotron X rays of energies in the range 4 to 20 keV: either as white beam or monochromatic, and either unfocussed or focussed. We have used collimators, of sub-micrometre cross-section, for white radiation [1]; and, more recently, monochromatic radiation (11.6 keV) together with a linear series of 14 compound refractive lenses, giving an elliptical focal spot size 6.0 μm by 7.2 μm, to image inclusions in natural and synthetic diamonds. Specimens were scanned on an X-Y stage and images were obtained both in transmission and by X-ray fluorescence energies characteristic of chosen metallic elements. The X-ray fluorescence spectra at each pixel were also recorded.
The diamonds were selected for the variety of their inclusions to test the imaging capability of scanning X-ray microscopy: four diamonds from the Finsch Mine (South Africa), one from Udachnaya (Siberia) and one from Orapa (Botswana), as well as some synthetic diamond grit particles. The Finsch diamonds were polished plates, 2–3 mm in thickness and 5 mm in diameter. One was a 'coated' stone with a clear core and a cloudy overgrowth containing numerous small black sulphide or graphite inclusions; one had a cloudy cube-shaped core; one was a twin (a 'macle') of peridotitic paragenesis containing purple chrome-rich garnet inclusions; and another was of eclogitic paragenesis which contained garnet inclusions as well as a pale olive-green cloudy region of tiny unidentified inclusions. We found that the cuboid growth sectors of this eclogitic diamond contained nickel.
The two other diamonds, a rounded dodecahedron of about 2 mm in diameter from the Udachnaya mine containing an inclusion of chromite, and an octahedron of about 2 mm in size from the Orapa diamond mine, containing a sulphide inclusion, were also selected for imaging experiments on the inclusions. Many inclusions were indeed imaged and the X-ray fluorescence spectra were recorded. These experiments demonstrated the power of scanning X-ray microscopy to identify non-destructively the various chemical elements contained in inclusions lying well within thick diamond specimens.
We thank Dr Jeff Harris (University of Glasgow) and Prof Simon Connell (University of Johannesburg) for the loan of the diamond specimens; and Dr Kawal Sawhney, Dr Manoj Tiwari and Dr Igor Dolbnya (Diamond Light Source) for help with the synchrotron experiments.

[1] Moore, M., *J. Phys.: Condensed Matter*, 2009, **21**, 364217 (15 pp).

Keywords: diamond, inclusions in minerals, X-ray imaging

FA5-MS40-P10

Hard X-ray diffraction scanning tomography with sub-micrometer spatial resolution.

Hervé Palancher[a], Rémi Tucoulou[b], Pierre Bleuet[c], Anne Bonnin[a,b], and Peter Cloetens[b], [a] *CEA, DEN, DEC, Cadarache, F13108 Saint Paul lez Durance, France,* [b]*ESRF, ID22/ID22Ni, BP220, F38043 Grenoble Cedex, France,* [c]*CEA, LETI, MINATEC, F38054 Grenoble, France*
E-mail: herve.palancher@cea.fr

To perform 3D crystallographic phases imaging inside polycrystalline single phase but also multi phases samples, a new method combining X-ray powder diffraction with scanning tomography has recently been proposed [1-3]. One major advantage of this technique (written here Xray Diffraction-Computed Tomography (XRD-CT)) is that contrary to others methods no *a priori* knowledge on the phases present in the sample (crystallographic structure ...) is required. The spatial resolution of this technique is directly linked to the beam size incoming on the sample and micron-scale resolution has already been demonstrated [1]. The capability of the method to reach higher spatial resolution and therefore to access nanomaterials characterization is linked to the focusing capabilities of the beamline. Since the XRD-CT technique is based on powder diffraction methods, Rietveld refinement can be partly included in the data processing just like for 2D-XRD. A previous study based on a quite similar approach for XRD-CT data treatment has been recently proposed [2]. We report in this paper the first attempt to perform XRD-CT measurements on the ID22NI hard X-ray nanoprobe of the European Synchrotron Radiation Facility (ESRF) with a beam size of 150×220 nm [4]. The studied sample is a small spherical (about 50 μm in diameter) annealed UMo particle and a multiphases interface buried about 5 μm under the surface has been especially characterized. Moreover the interest of Rietveld method for analyzing the XRD-CT data will be evaluated and the possibility to derive from such an approach the weight fraction of the various phases inside each voxel will be discussed. Finally, the advances provided by this experiment on our understanding of the UMo/Al metallurgy will be presented.

[1] Bleuet, P.; Welcomme, E.; Dooryhee, E.; Susini, J.; Hodeau, J.L. and Walter, P.; *Nature Materials*, 2008, 7, 468. [2] De Nolf, W.; Janssens, K.; *Surface and Interface Analysis* published online 10Nov. 2009. [3] Artioli, G.; Cerulli, T.; Cruciani, G.; Dalconi, M.C.; Ferrari, G.; Parisatto, M.; Tucoulou R; *Anal. Bioanal. Chem.*, 2010, DOI: 10.1007/s00216-010-3649-0. [4] Mokso, R.; Cloetens, P.; Maire, E.; Ludwig, W.; Buffiere, J. Y.; *Appl. Phys. Lett.*, 2007, 90, 144104.

Keywords: diffraction tomography, 3D-characterization, sub-micrometer resolution