

work for XRD analysis using mathematic functions to simulate the XRD peaks and to find the solution for structures. This work is based on i) an XRD peak is consisted of five basic elements [2] such as, peak position, maximum intensity, full width at half maximum, shape coefficient and asymmetry, and the integrated intensity and integrated width can be produced from them; ii) an XRD peak can be well described by those functions, nowadays, such as: the Voigt, the pseudo-Voigt and the Pearson VII functions. Comparing the experimental peaks of normal XRD (line source) with those of micro XRD (point source) it reveals, for the sake of five basic elements, that i) the intensity from micro XRD is as 20-time strong as that of normal XRD on the equivalent conditions, e.g. the same sample from the same illumination area and ii) the resolution of micro XRD is as half low as normal XRD analysis, iii) the peak shapes of micro XRD are super wide and round at top and super narrower at bottom, iv) there is no difference in position between normal and micro XRDs and v) nearly symmetry in shape of the micro XRD peak on the equivalent optic conditions. In the normal XRD system, the fixed divergence optic path causes a different illumination length (area) on lower and higher diffraction angle sides of a reflection that leads the different intensities on two sides of a reflection and thus induces the asymmetry of a peak. Due to nearly no divergence the micro diffraction system produces an equal illumination on both lower and higher diffraction angle sides of a reflection and results in symmetry peak in shape. Depending on the convergence optics the highest resolution of normal XRD reaches a minimum width of $0.045^\circ \Delta 2\theta$, e.g. the resolution of the X'Pert Pro diffractometer. However, for the micro diffraction system, it is not the convergence optics and thus reduces the resolution of a peak. It is deduced from the shape characteristics of a micro diffraction peak that a band of quartz's reflections (212), (023), (301) and their $K\alpha_2$ doublets from normal XRD (in the range of $67-69^\circ 2\theta$ Cuka radiation and often shows five independent peaks) will merge into corresponding four or three or two or even one micro diffraction peak if the peak width of those quartz reflections from normal XRD be >0.0777 or >0.0836 or >0.0861 or $>0.1625^\circ \Delta 2\theta$ respectively. This is verified by quartz sample measured with the micro diffraction system. It is concluded that the micro diffraction peak possesses a super symmetric Gaussian distribution in shape (shape coefficient $Sc_{\text{micro}}=1.015$; note: $Sc_{\text{normal}}=0.63-0.94$) and with a double equivalent width whilst the normal XRD peak is of an asymmetric shape in different variations from the Gaussian extreme to the Lorentzian extreme mostly.

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Keywords: peaks, microdiffraction, function

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Simultaneous imaging of radiographic and crystallographic information. Jürgen Bauch^a, Dietmar Wünsche, Frank Henschel, Hans-Jürgen Ullrich, *Institute of Materials Science, Technical University Dresden, Germany*
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Real structure characterisation of bulk single crystals or large grain polycrystals is often made by X-ray diffraction, in which the intensity distribution of the diffracted beam is imaged in

back-reflection. The X-ray topographic method delivers information about the distribution of crystals defect in the surface and over a small depth within the sample. In many cases it is also important to investigate the real structure over the whole volume of a single crystal (dislocation density and distribution, small angle grain boundaries, lattice plane distortion, macroscopic and microscopic inclusions). For this transmission methods are suitable only. Due to the typical thickness of a sample hard X-rays or neutron beams can be used only. If a high spatial resolution is desired then it is appropriate to use hard X-rays emitted from a micro or "nano" focus X-ray tube. With this it is possible to observe macroscopic and microscopic defects by X-ray projection microscopy or by micro-computer tomography (μ CT). On the other hand, the diffracted hard X-radiation delivers real structure information from the inside of the crystalline sample. A report is given about the parallel measurement of diffraction and shadow microscopy information using divergent hard X-rays [1]. As part of this, the equipment and its components as well as the production of images will be discussed, along with some highlighted measurements. We thank the Deutsche Forschungsgemeinschaft for their sponsorship.

[1] Bauch J., Ullrich H.-J., Böbling M., Lupascu D.C., *Deutsche Patentschrift DE 10 2008 008 829*

Keywords: X-ray, XRD in transmission, real structure imaging

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Automatic detection and analysis of conic X-ray diffraction lines. Jürgen Bauch^a, Frank Henschel^a, Matthias Schulze^b, ^a*Institute of Materials Science*, ^b*Institute of Photogrammetry and Remote Sensing, Technische Universität Dresden, Deutschland*
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The presented method demonstrates a first step in the development of a high resolution "Residual stress microscope". It has been implemented but is not exclusively used for the KOSSEL technique and the "X-ray Rotation-Tilt Method" (XRT). Through the implementation of as far as possible automated procedures the presented method allows rapid access to a diverse evaluable data base of many X-ray diffraction images. Thus, there is now the possibility of systematic studies of materials science based basic phenomena, such as smeared or double reflection maxima and local maxima along a diffraction line. An essential component is the fully automatic detection of these reflections in form of conic sections (quadratic curves). This is done with the involvement of modern methods of digital image analysis and processing, for instance the 3D Hough transform. In addition to the detection of the inexact location of diffraction lines, there is also the registration of reflection micro structure with subpixel accuracy and other curve parameters with associated adjustment calculus. The thus obtained data can be used, inter alia, for the calculation and output of the precision strain- and residual stress tensor. We thank the Deutsche Forschungsgemeinschaft for their sponsorship.

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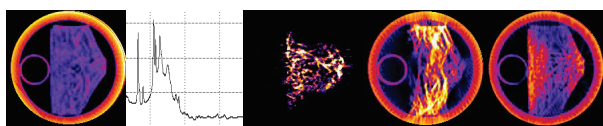
Keywords: X-ray diffraction analysis programming, KOSSEL diffraction, XRT technique

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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, ^aInstitut Néel, CNRS-UJF, 38042 Grenoble, France, ^bESRF, BP 220, 38043 Grenoble, France, ^cCEA/LCPO & CEA-LETI, Grenoble 38054, France. ^dUniv Aveiro, Dept Fis, Ciceco, P3800 Aveiro, Portugal
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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 $2 \times 1 \mu\text{m}^2$ and $100 \times 100 \mu\text{m}^2$ 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.

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Keywords: diffraction-tomography, texture, fullerenes

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Conditions for reception of x-ray monochromatic bunches of the maximum intensity in geometry Laue.

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In the presented work dependence of absolute value of intensity of monochromatic x-ray radiation, diffracted from a direction of an 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.

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Probing inclusions in diamonds with fine beams of synchrotron X rays Moreton Moore^a, Rais

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