is an extension of the widely used powder diffraction based 1D-PDF technique. It is obtained by Fourier transformation of single crystal (diffuse) scattering. Contrary to 1D-PDF it provides not only information about the length, but also about the spatial orientation of real inter-atomic vectors. The 3D-PDF method allows employing techniques that are difficult to apply in the case of powder diffraction. Complexity of 3D-PDF maps may be strongly reduced by filtering out information that is either already known or not of interest. As an example Bragg scattering from the usually well-known average structure may be eliminated before calculating the 3D-PDF what strongly enhances visibility of disorder information [1]. Further, independent disorder phenomena may be separated in reciprocal space, if they show distinct sets of diffuse scattering, and/or in PDF space, if the orientation of inter-atomic vectors allows distinguishing different kinds of disorder e.g. intra- and interlayer disorder. An instructive example for demonstrating the power of 3D-PDF analysis is diffuse scattering from quasicrystals, which certainly belongs to the most complex disorder problems. It will be shown that the 3D-PDF method allows understanding of extremely complicated diffuse scattering from decagonal Al-Cu-Co and Al-Co-Ni quasicrystals by multiple reduction of complexity in reciprocal and PDF space [2,3].

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Keywords: pair distribution function, diffuse scattering, quasicrystals

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Nanostructure of silver-free photochromic glasses studied by anomalous small angle X-ray scattering

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Cuprous halide nanocrystals, embedded in a glassy matrix are of interest with respect to their photochromic behaviour. A silver-free photochromic glass was prepared using a $14.2Na_2O$-$6.0Al_2O_3$-$26.6B_2O_3$-$53.2SiO_2$ base glass doped with small amounts of Cl, Br, Cu, Cd, and Sn ions. During isothermal heat treatments at T = 600 ℃, small liquid droplets of CuX precipitate resulting in $CuCl_{0.4}Br_{0.6}$ nanocrystals after cooling. It is known, that both Cd and Sn ions have a large influence on the photochromic properties and on the sizes of the nanocrystals. But the structural arrangement of the Cd and Sn ions in- or outside the nanocrystals is not known. In order to investigate the influence of Cd and Sn on the precipitation process and to understand the growth and growth delay processes, anomalous small angle X-ray scattering (ASAXS) experiments have been performed. The X-ray energy has been tuned near below the K-absorption-edges of Cu, Br, Cd and Sn giving rise to a variation of the atomic scattering factor of the corresponding element. The result of the simultaneous fits of all curves assuming two different models for the particles will be presented. Both models, poly-disperse core-shell and diffusion zone surrounding spherical crystals, lead to the same conclusions. The crystalline core consists of the element Cu, Cl and Br. Cd and Sn are concentrated in a shell surrounding the nanocrystals. These structural models together with the measured viscoelastic behavior of the glass can explain the growth stop of the crystals after annealing of about 60 min at 600 ℃, knowing from previous SAXS studies.

Keywords: ASAXS, photochromic glasses, nanocrystals

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Can amphipols be used to crystallize membrane proteins?

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'Amphipols' are a family of specially designed amphipathic polymers that can substitute to detergents at the hydrophobic transmembrane surface of membrane proteins (1,2). Amphipol-trapped membrane proteins are soluble in aqueous solutions in the absence of detergent, in their native state, and, as a rule, much more stable than in detergent solutions (1-4). Because amphipols are very mild surfactants, they provide a favorable medium in which to fold to their native state denatured membrane proteins (5), including G protein-coupled receptors overexpressed as inclusion bodies (6). Amphipol-trapped membrane proteins can be studied by NMR (7), electron microscopy (8), and most spectroscopic and other biophysical methods (2,3). Because the protein/polymer association is irreversible, trapping with a functionalized amphipol will functionalize the protein without having to modify it chemically or genetically (9). Thus, trapping with a biotinylated amphipol makes it possible to attach the protein to a solid support for the purpose of screening for biological partners, ligands, drugs, antibodies etc. (10). Whether amphipols can be used to crystallize membrane proteins remains, however, an open question. An update will be presented of where we stand relative to this particular application and what the perspectives seem to be.

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Crystallisation of the calcium pump of skeletal muscle sarcoplasmic reticulum

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