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Disorder and Diffuse X-ray Scattering in Colloidal and Photonic Crystals. Andrei V. Petukhov, van 't Hoff laboratory for physical and colloid chemistry, Debye Institute for Nanomaterials Science, Utrecht University, The Netherlands.

E-mail: a.v.petukhov@uu.nl

Colloids are particles of up to about a micron in size, i.e. thousands times larger than ordinary atoms. Despite this drastic size difference, colloids are able to spontaneously form crystals and liquid crystals, just like atoms and molecules do. Colloids are therefore considered as important models, which allow mimicking the essential physics of the nucleation and growth, phase transitions, gelation and glass transition on more convenient spatial and temporal scales. Colloid self-assembly is also used for promising applications such as photonics. High penetration power of hard x-rays, intrinsically low contrast and the possibility of in-situ investigations make x-rays very suitable to study self-organization in colloidal suspensions. However, because the colloids are huge compared to the x-ray wavelength, x-ray diffraction can be observed only at very tiny angles, $< 10^{-3}$ radian, which makes x-ray diffraction very challenging.

In this contribution it will be shown that the challenge can be met by using synchrotron sources and refractive x-ray optics. Angular resolution down to $\sim 10^{-6}$ radian can be achieved, which allows revealing fine details in the diffraction patterns at ultra-low angles [1]. One of the illustrations will be the microradian x-ray diffraction in random-stacking sedimentary crystals of hard colloidal spheres [2]. Diffuse x-ray scattering along the Bragg rods, which originate from stacking disorder, will be discussed in detail. In addition, effect of dynamic (multiple) diffraction, which leads to the appearance of additional 'forbidden' Bragg rods, will be demonstrated. We then shall move to the convectively-assembled crystals, where the primary crystal structure is cubic. Still, stacking disorder is also present here but in a form of pairs of hcp planes, as it can be seen in the distribution of the diffuse x-ray intensity along the Bragg rods [3].

Finally, a couple of examples of the application of microradian x-ray diffraction to colloidal liquid crystals will be presented [4]. In particular, we shall discuss the undulation fluctuations in the smectic phase of goethite nanorods, which lead to diffuse 'tails' of the smectic Bragg peaks. It will be shown that in contrast to the usual splay-type layer undulations studied so far, the goethite smectic phase shows undulations of a sliding type, which does not lead to the Landau-Peierls instability.

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Real-structure effects of luminescent layered oxonitridosilicates. Oliver Oeckler, Markus Seibald, Juliane A. Kechele, Florian Stadler, Tobias Rosenthal, Hans Koss, Wolfgang Schnick. Department of Chemistry, LMU Munich, Germany.

E-mail: oliver.oeckler@gmx.de

Oxonitridosilicates have received much attention owing to their suitability as host lattices for rare-earth doped phosphors in light-emitting diodes.[1] Their crystal chemistry is remarkably complex and characterized by numerous real-structure effects that can only be elucidated by a combination of diffuse X-ray diffraction and HRTEM techniques. The situation is further complicated as, in many cases, the materials are microcrystalline and/or contain several sometimes closely related phases.

The luminescence properties of the layered compounds $MSi_2O_2N_2$ ($M = Ca, Sr, Ba$) are particularly promising.[2,3] Their layered silicate substructures exhibit highly condensed $SiON_3$ tetrahedra interconnected by N^{3-} atoms. These layers are interconnected via cations coordinating terminal O atoms of the tetrahedra. Both the cation arrangement and the silicate layers are highly pseudosymmetric. This fact gives rise to numerous real-structure effects such as twin and anti-phase boundaries and intergrowth phenomena. Whereas HRTEM has revealed the structural features of $SrSi_2O_2N_2$,[4] and a combined approach including neutron diffraction proved necessary to analyze $BaSi_2O_2N_2$,[5] the analysis of diffuse X-ray scattering allowed to quantify the ratio of twin and anti-phase boundaries in solid solutions $(Sr,Ba)Si_2O_2N_2$. This is essential to understand the excellent luminescence properties of mixed crystals, which are influenced but not deteriorated by the high concentration of domain boundaries.

In addition to disorder, $Sr_5Al_{5-x}Si_{21-x}N_{35-x}O_{2+x} \cdot Eu^{2+}$ ($x \approx 0$) is characterized by two types of silicate layers (containing dreier and sechser rings, respectively) that form a series of both commensurate or incommensurate intergrowth compounds. Different sequences of edge and vertex sharing tetrahedra determine the lattice translation of the sechser ring layer, on which the dreier ring layer imposes a modulation wave and vice versa. Whereas the dreier ring layer is 2D long-range ordered, the other subsystem often exhibits no strict periodicity. This means that there is a smooth transition from modulation effects to disorder. Whereas diffraction patterns allow to assess the correlation length and the metrics of the intergrowth, the local atom arrangements were derived from simulations of HRTEM data. Despite the complex structure, the cation coordination varies only slightly, which explains the rather sharp emission of Eu^{2+} .

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Keywords: silicate structure determination, diffuse X-ray scattering, electron microscopy of crystals