Keywords: coordination crystal chemistry, carbonyl-bridged nitrogen heterocycle, supramolecular assemblies

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Molecular recognition and self-organization of three-way DNA junctions and supramolecular helicates

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Helicates are mixed metallic-organic structures with three-fold symmetry that exhibit high affinity for DNA. We have crystallized several helicates in complex with palindromic DNA oligomers and solved their structures. The analysis reveals a DNA three-way junction (3WJ), where the helicate occupies the central cavity of the junction. The shape complementarity between both is extraordinary. We describe the recognition of the three-way junction by the helicate in detail. The interactions in the complex consist of pi-pi interactions between the DNA bases and the central aromatic region of the helicate and electrostatic interactions between the Fe(II) centres and the phosphate backbone. In addition, we describe the macroscopic features of the crystal structures that we have determined. The crystals are porous materials that are formed as a result of the incorporation of additional helicate molecules at the extremes of the DNA arms. A three-dimensional, chicken wire-like network is formed through alternation of 3WJ's of different topologies. The chirality of some of the helicate centres modulates the overall topology of the crystal network. We suggest that helicate-bound 3WJ's may constitute a valuable addition to the existing tools and structural modules for the design and assembly of DNA-based nanomaterials.

Keywords: self-organization, nanomaterials, single crystal

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Analysis of residual stresses induced by surface processing: Angle *vs.* energy dispersive diffraction

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Mechanical, thermal and/or chemical surface processing as well as coating introduce residual stresses in the near-surface zone of technical parts, which may influence the material properties significantly. Among the methods for residual stress analysis diffraction techniques take up a unique position, because they allow for non-destructive and phase-selective evaluation of stress distributions from the surface down to the volume of the material. Compared to X-ray stress analysis (XSA) performed in the angle-dispersive (AD) mode of diffraction which has a very long tradition, energy-dispersive (ED) stress analysis is a comparatively young method. The advantages of ED synchrotron diffraction are the short measuring times allowing for fast in-situ studies and the multitude of diffraction lines recorded in each spectrum, which contain additional information for depth-resolved XSA. The absolute resolution of ED experiments being mainly controlled by the detector system, however, is lower than that attainable by AD methods. Assets and drawbacks of AD and ED XSA techniques are discussed with respect to their ability to detect non-uniform residual stress fields in the near surface region of polycrystalline materials. It will be shown that there is no universal method which solves all problems related to X-ray stress analysis at once. The decisive parameter which adjudicates on the applicability of a method to a special problem is the ratio of the sampled volume to the steepness of the expected stress gradient. This general rule applies for all methods independently of the diffraction mode (AD or ED) and the way used for depth resolution (Real- or Laplace space approach). To succeed in case of complex systems the use of complementary methods is recommended.

Keywords: residual stress analysis, synchrotron radiation, X-ray diffraction techniques

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X-ray line profile analysis for the characterization of nanostructured materials

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For the characterisation of micro- and nanostructures in bulk as well as in loose powder materials the X-ray Line Profile Analysis (XPA) has proven to be an excellent method. According to the kinematical theory of scattering, diffraction profiles are the convolution of the size and distortion profiles [1]. Size broadened profiles can be described by assuming (i) a size distribution function and (ii) the shape of crystallites or of coherently scattering domains. From a log-normal size distribution function f(x), which is given by the median m and the variance σ, weighted average crystallite sizes can be evaluated [2]. In the case of strain broadening the major task is the description of the mean square strain. Phenomenological and also dislocation models have been designed to describe the diffraction vector dependence of the mean square strain [3, 4]. This way the density and distribution of dislocations can be determined even for very high densities. Further improvements enable the verfication of planar faults such as stacking and twin faults in parallel to the hitherto parameters. A whole profile fitting procedure, previously worked out for determining the dislocation structure and crystallite size distributions, is extended for planar fault by including these parameter into the evaluation algorithm [5]. The universal character of the method are documented by several examples.

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