Although the obtained crystallite dimensions and morphology are affected by the approximations of the diffraction pattern model used in the refinement, the technique described in the present work is always valid. Crystallite dimensions, however, approximate more to their real values, as the model used for the Rietveld refinement is improved.

Keywords: Rietveld refinement, crystallite dimensions, Delaunay triangulation

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X-ray powder microdiffraction and its limits in forensic practise

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X-ray diffraction is an important technique of forensic practise for accurate phase analysis of soil, pigments, explosives, drugs, etc. Recently, X-ray Powder Microdiffraction (micro-XRPD) has been applying predominantly, allowing analyses of very small samples. The analysed area is approaching to a size of surfaces examined by microscopic techniques, light microscopy, SEM/EDS, etc., routinely used in forensic practice. Combination of these techniques provides complementary information. Micro-XRPD allows in the forensic field a direct phase analysis recovered from traces, for which XRPD was not feasible. To employ micro-XRPD for microscopic fragments and abrasions it was necessary to carry out tests of different ways of sample fixation allowing the performance of other analyses by different methods (SEM/EDS, optical microscopy, FTIR, etc.) on the same carrier. These sample treatment eliminate either the possibility of loss or trace contamination. Classical aluminum specimen mounts for SEM with carbon tape, zero-background silicon sample holders, foils designed for XRF sampling, etc., were analysed. Each of different fixation methods brings some advantages and some drawbacks for each kind of analysed traces. Another limiting factor tested for micro-XRPD is the size of monocrystalic areas in a sample. In the case of samples containing micro/nano particles and nanocomposites plays a pivotal role the issue of detection limits for different types of these materials and their comparisons with different configuration limits of classical XRPD. Both mixture models and real materials from different areas were tested.
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Keywords: forensic microanalysis, microdiffraction, nanophases

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Analysis of atomic structure and structural imperfections of ZnTe and (Zn,Mn)Te nanowires

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ZnTe and (Zn,Mn)Te NWs were grown on GaAs substrates by molecular beam epitaxy via a vapour/liquid/solid mechanism (VLS) where nano-sized droplets of a gold-based eutectic act as catalysts [1]. The morphology, atomic structure and chemical composition of the NWs were investigated by transmission electron microscopy (TEM) [2]. The wires grew along the <111> directions pointing out of the (001) GaAs. The length of the wires amounts to some microns depending on the growth time. The mean diameter ranges between 30 and 60 nm depending on the size of the gold droplet located at the tip of the NWs. The NWs are single crystals. The majority of the NWs exhibit numerous two-dimensional crystal defects (stacking faults, microtwins) with only a few {111} monolayers sequence perpendicular to the NW axis as revealed by high-resolution TEM. The different types of defects were analysed in detail. The NWs consist of a core-shell structure as detected by electron energy loss spectroscopy (EELS). The shell of the NWs is formed by ZnO. The gold spheres at the tip of NWs additionally contain gallium, zinc, and tellurium. The gallium is incorporated during the initial formation of the eutectic droplets at the GaAs substrate. The distribution of the Mn along and across the NW in (Zn,Mn)Te NWs is homogeneous as detected by EELS measurements. The formation process of the NWs can be understood as a two-step process. The first step is the one-dimensional growth along the wire axis by consuming all the material deposited near the droplet. In a second step, facets are formed due to lateral growth of the NW.
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Keywords: crystal defects, nanowires, TEM characterization

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Edgeworth-series description of anisotropic microstrain broadening in powder-diffraction patterns

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The diffraction effects of non-Gaussian microstrain distributions within the Stokes-Wilson approximation are described by anisotropic Edgeworth series, which can - for each reflection hkl - be quantified by the 3rd, 4th ... Nth cumulants of the microstrain distribution projected on the diffraction vector of each reflection hkl. The diffraction-vector (hkl) dependence of these Nth cumulants can be described by 2Nth-rank tensors. The situation considerably simplifies in case of univariateness of the microstrain distribution, leading to equal (or inverted) shapes of the line-broadening contribution for all different hkl reflections. The model was applied to re-evaluate previously presented X-ray powder diffraction patterns of two somewhat inhomogeneous epsilon-iron-nitride powder batches, epsilon-FeN0.433 [1] and epsilon-FeN0.407 [2]. The data had revealed [1, 2] anisotropic and partly asymmetric microstrain(-like) broadening due to the N-content dependence of the lattice parameters of these hexagonal iron nitrides [3]. The specific origin of the microstrain leads to univariateness of the microstrain distribution [1, 4]. As a result of the data re-evaluation using the model of anisotropic Edgeworth series for description of the observed microstrain broadening, Edgeworth series-type probability-density functions for composition of these two powders have been determined, quantifying the inhomogeneity of the two powder batches, respectively.
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