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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Keywords: powder diffractometry, X-ray line profiles, microstructure characterization

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Cathodoluminescence characterization of tridymite and cristobalite

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Cathodoluminescence (CL) spectra of tridymite and cristobalite have blue broad peaks around 430 and 400 nm, respectively, both of which can be assigned to self-trapped exciton (STE) localized to [AlO_4/M+]0 defect. CL intensities of these blue spectral peaks decrease with extending exposure time of electron irradiation as a short-lived luminescence observed in quartz CL, whereas quartz shows a less decrease of CL intensity compared with these minerals. Cristobalite has a higher CL intensity reduction rate during irradiation compared to tridymite. The irradiation at low temperature results in more rapid decay of CL emission, while quartz shows no obvious change in similar temperature. A confocal micro-Raman spectroscopy on the electron irradiated surface of these minerals reveals the amorphization caused by a penetration of electron beam in the surface layer with a depth of 4 to 6 micron meters. This suggests that such structural destruction diminishes the activity of CL emission centers related to STE localized to [AlO_4/M+]0 defects by migration of monovalent cations associated with exchanged Al in the tetrahedral site. Both samples present a considerable reduction of their CL intensities at higher temperature, suggesting a temperature quenching phenomenon. The activation energy in quenching process was evaluated by a least-square fitting of the Arrhenius plots, assuming the Mott-Seitz model. The result implies that the energy of non-radiative transition in this process might be transferred to lattice vibration as phonon in two different manners. This energy transfer might be related to different irradiation response of the CL with a change of sample temperature.

Keywords: cathodoluminescence, tridymite, cristobalite

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Strain profiles and crystallographic defects in 6H SiC implanted with 2 MeV As ions

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Silicon carbide is a modern semiconductor material with physical properties differing very much from the other dominating in electronic industry. The important method used in the technological applications of SiC is the ion implantation. The structural changes caused in SiC by this method are not yet very well known, especially in case of heavier ions. In the present work the ion implanted layers were produced in highly perfect (00.1) oriented 6H SiC wafers. The implantations were performed with 2 MeV As^+ ions to a number of fluences in the range from $6\times10^{12}cm^{-2}$ to $2\times10^{14}cm^{-2}$. They samples were examined before and after implantation with a number of synchrotron X-ray diffraction methods and Rutherford backscattering/channeling method. The X-ray methods included the investigation of local rocking curves recorded with a 50 × 50 μm^{-2} probe beam and white beam Bragg case section and projection topography. The synchrotron topographic examination performed before the implantation indicated well resolved individual dislocations of the density smaller than 10^3cm^{-2}. It was found with the use of numerical simulation that majority of the dislocations were the screw ones located along [00.1] direction. The implanted layers provided distinct interference effects both in the rocking curves and Bragg-case section topographs (strain modulation fringes). The presence of distinct interference maxima was essential for evaluation of the strain profile by fitting the theoretical rocking curves. The evaluated strain profiles approximated by browsed Gaussian curve were similar to the distribution of point defects calculated with SRIM2008 code. The profiles were similar to the defect distribution determined from the channeling measurements.

Keywords: silicon carbide, ion implantation, X-ray strain determination

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Observation of dislocation in 4H-SiC by means of weak-beam and plane-wave X-ray topography

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Dislocations in 4H-SiC wafers have been studied using X-ray topography in Bragg-case using synchrotron radiation X-ray beam. Our standard geometry was grazing-incidence extremely asymmetric and diffraction vectors were 11-28 and the X-ray wavelength was 0.15 nm. In order to clarify the dislocation nature, the topographic images were compared with those taken under the weak-beam condition. The basal-plane dislocation images became much narrower in width and they were decomposed to separate lines under the weak-beam condition. The threading-screw dislocations showed changes in their shape and contrast as the crystal set was tilted from the rocking-curve peak, and finally the characteristic images near the dislocation core were observed under the weak-beam condition. Plane-wave topography was also performed to examine the dislocation images in detail. The monochromatic beam form Si 111 double-crystal monochromator was collimated using Si 331 asymmetric reflection, and topographic images at g=0008 from the sample crystal were recorded, and the wavelength was 0.16 nm. Strain contour due to the strain filed around defects were observed, and some typical images for threading screw-dislocations were observed. We discuss the dislocation nature based on these experimental results and theoretical calculations.

Keywords: X-ray topography, dislocation, SiC