and 800 μm capillaries, and counting-time 2000 and 400 seconds/ step respectively. The results of this research will be used in routine forensic investigations in the Prague Institute of Criminalistics.

Keywords: X-ray diffraction; microdiffraction; forensic science

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Preferred Orientation and the Structure Analysis Of Polycrystalline Materials. Jürgen Grässlin[a], Lynne B. McCusker[a], Christian Baerlocher[a], Fabia Gozzo[b], Bernd Schmitt[b]. [a]*Laboratory of Crystallography, ETH Zurich, CH-8093 Zurich, Switzerland.* [b]*Swiss Light Source, PSI, CH-5232 Villigen, Switzerland.*
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If the crystallites in a polycrystalline sample are oriented, the intensity of a reflection will vary as a function of the orientation of the sample in the X-ray beam. This means that even if two reflections overlap in a conventional powder diffraction pattern (i.e. have the same *d*-value), their intensities are likely to vary differently as a function of sample orientation, so their individual intensities can be deduced if data are collected at different sample orientations. It has been shown that this principle can indeed be exploited to obtain more single-crystal-like data from a polycrystalline material [1]. Although the initial study was performed in reflection mode, it was soon realized that a transmission geometry offered several advantages and the experiment was adapted accordingly. In particular, the problem of sample homogeneity was eliminated (the sample is bathed in the X-ray beam), the severe correction of the data for the sample tilt was no longer necessary, and less synchrotron beamtime was required. To start with, a 2-dimensional image plate detector was used, but the resolution of the diffraction patterns, both in d_{min} (2θ range) and in peak width proved to be a limitation [2]. To overcome this, the experiment was changed once again to accommodate the 1-dimensional Mythen I Si-microstrip detector that was available on the Materials Science Beamline at SLS [3,4]. Now, a new version of this detector, Mythen II, has become available, and further optimization of the experiment can be undertaken. The detector now has a 2θ range of 120˚ (*vs.* 60˚), has a much larger dynamic range, and is not plagued by random dead and hot channels. Consequently, a different, more efficient, data collection strategy can be employed. Improvements in the data analysis software *Maud* [5] have also made it possible to reduce the data collection time. Constant 5˚ steps in the sample rotation (φ) and tilt (χ) angles are no longer required, so the number of sample orientations to be measured can be reduced from 1368 to 302 without sacrificing information content. The first measurements with the new detector and the new data collection strategy have now been performed. Textured samples of phlogopite mica and the aluminophosphate $AlPO_4$-17 (**ERI** framework type), with known crystal structures, and of a niobium silicate with an unknown structure have been measured. Preliminary analysis of these data show that sensible orientation distribution functions can be derived, and the full intensity extractions are in progress. The crystal system of the niobium silicate was ambiguous because unit cells in several different crystal systems (hexagonal, orthorhombic, monoclinic) were possible. The texture analysis has now shown that only the orthorhombic unit cell is consistent with the measured pole figures.

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Keywords: preferred orientation; structure determination; X-ray powder diffraction

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Effects of the Ferroelectric Domain Structure of PZT Ceramics on Powder Diffraction. Kristin A. Schoenau[a], Michael Knapp[b], Matteo Leoni[c], Hartmut Fuess[a]. [a]*Materials Science, Darmstadt University of Technology, Germany.* [b]*CELLS, Barcelona, Spain.* [c]*Dept. Materials Engineering and Industrial Technologies, University of Trento, Italy.*
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Ferroelectric lead zirconate titanate solid solutions, $PbZr_{1-x}Ti_xO_3$ (PZT), are frequently used in industrial applications exploiting the reaction of both the lattice and the domain structure to an applied electric field. Diffraction is a powerful and necessary tool to be able to understand materials reaction and to separate these two effects through analyzing intensity changes and shifts in peak position under electric field.
Highest strain is found for compositions at the morphotropic phase boundary (MPB) between the tetragonal and rhombohedral phase field. Discussions on its origin involved a coexistence of tetragonal and rhombohedral structures as well as the existence of a monoclinic phase [1]. Recent studies using high-resolution synchrotron x-ray powder diffraction in combination with TEM and EPR at ambient temperature [2, 3] were able to correlate XRD observation with a nanodomain structure. Theoretical approaches using Martensitic theory describe these observations with strong coherence effects between ordered nanodomains in diffraction experiments [4].
In XRPD anisotropic peak broadening effects and asymmetries in line shape for distinct hkl are already observed for single phase tetragonal material with a large domain size. But so far the asymmetry and intensity observed in between split reflection pairs have been attributed to diffuse scattering from strained domain walls [5], which is not in line with TEM observations [6].
We therefore analyze diffraction data of single phase tetragonal and rhombohedral PZT in the vicinity of the MPB recorded in transmission mode at the beamline B2, Hasylab, Hamburg Germany, using Rietveld refinement and size-strain analysis to be able to determine a sound basis for analysis of diffraction data of morphotropic PZT samples.

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