MS50-P6 Two- and three-dimensional analytical X-ray techniques for analysis of crystalline materials

Hans te Nijenhuis,[a] Fabio Masiello,[a] Detlev Götz,[a] [a]*PANalytical B.V., Lelyweg 1, 7602 EA Almelo, The Netherlands,*
E-mail: hans.te.nijenhuis@panalytical.com

X-ray diffraction is a widely used technique for the analysis of crystalline materials. Most of the materials investigated are polycrystalline and can be analyzed with the use of standard optical configurations, such as the Bragg-Brentano geometry. However, in modern materials analysis the focus is more and more directed towards thin films and single crystals with a high degree of perfection. Commonly, the crystal structures of these materials are known, and more advanced information about the crystalline quality is required to understand the physical characteristics of the material. Since these materials typically do not fulfill the requirements for the standard measurement geometries, other X-ray optical configurations are required to examine and visualize the fabric, defects and orientation.

The introduction of the latest generation of two-dimensional (area) X-ray detectors have created new possibilities for the materials scientist to analyze nearly perfect materials. The high dynamic range and the high spatial resolution of these detectors make it possible to reveal crystallographic information that was previously inaccessible due to the high intensities and the small line widths of the reflections measured.

As an example of the application of modern diffraction techniques used to examine (nearly) perfect materials we have investigated potash alum crystals. These crystals were grown from an aqueous solution under nearly equilibrium conditions. Therefore well-established crystal faces are observed, that can be used to directly relate the external morphology to the internal crystal structure. The main orientation of the crystal lattice could be determined from large area reciprocal space mapping. Using X-ray computed tomography techniques a three-dimensional reconstruction of the morphology of the crystal is obtained. With the use of the orientation matrix obtained from the reciprocal space map, the crystal faces can be indexed. The internal defect structure in the material was revealed by X-ray topography.

The combination of the information obtained in different experimental X-ray analytical configurations is used to give a complete description of the structural aspects of the crystals.

Keywords: computed tomography; reciprocal space mapping; topography