Poster

The effect of sample displacement in X-ray powder diffraction measurements with laboratory diffractometers

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Sample displacement is one of the most significant aberrations that affect the results of X-ray powder diffraction (XRPD) experiments. It can lead to an incorrect determination of d-spacings and lattice parameters, or to wrong materials found in phase identification analysis. Modern laboratory diffractometers provide options for minimizing the displacement using accurate sample positioning and dedicated alignment procedures. Despite this, errors caused by displacement are still often observed due to issues with the preparation of powder samples or to solid samples with dimensions that cannot be accommodated by the diffractometer. Most textbooks about powder diffraction, e.g. [1-4], include a description of this effect and software packages [5,6] apply corrections to the positions of diffraction peaks to either account for the known sample displacement or to estimate it. These corrections are often approximate and can only be applied for minor displacements in the order of a few hundred micrometers.

In this contribution, the effect of sample displacement in X-ray powder diffraction experiments with laboratory diffractometers is revisited and new expressions are derived for several commonly used experimental configurations, including Bragg-Brentano parafocusing geometry and flat-plate transmission geometry. The results presented here allow the analysis of data from samples with relatively large displacements (Fig. 1). This may open the possibility to study samples with dimensions that are difficult to accommodate with the sample-handling capabilities of standard laboratory diffractometers.

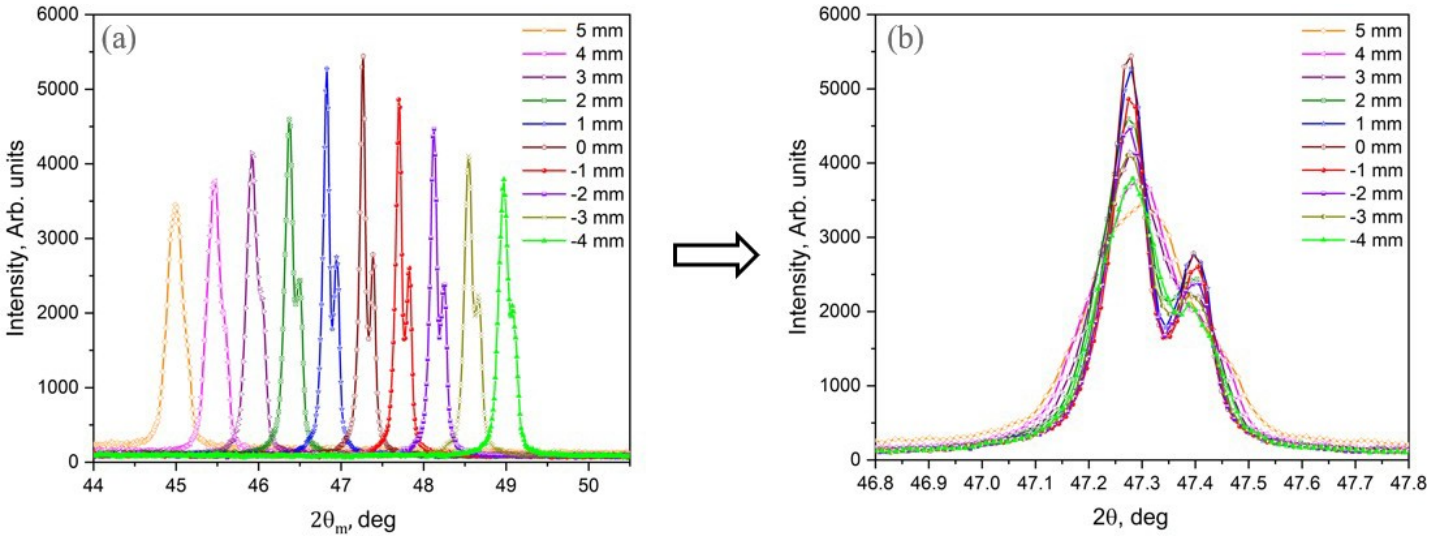

Figure 1. Diffraction peaks measured for various sample displacements before (a) and after (b) correcting the peak positions.

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