Oral Contributions

[MS16] X-rays and electrons: joining forces

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[MS16-01] Automated electron Diffraction Tomography (ADT) and X-ray powder diffraction for structure characterization of layered materials

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Layered materials attract increasing attention not only from the point of fundamental crystallography due to their structural diversity, but also due to their numerous industrial applications, for instance as gas storage systems or battery elements. Structural characterization is an essential key for understanding and controlling the desired properties. Layered materials have intrinsic features which turn their structure analysis into a challenging task. Large crystals suitable for singly-crystal X-ray analysis with exactly the same internal structure as fine powders can rarely be grown. Due to the internal construction of layered systems, the crystals predominantly have platelet on needle-like morphology causing problems with preferred orientation during the powder X-ray data collection. The systems are typically polyphasic, thus troubling the powder diffraction data analysis, and finally, they often show disorder in the stacking sequence. All above mentioned points make structural analysis of layered materials a complex mission demanding for a combination of advanced methods. One of the most beneficial approaches to the structure analysis of layered materials is the combination of electron diffraction tomography (Automated Diffraction Tomography – ADT [1-3]) and X-ray powder diffraction method [4-5]. The interaction of these complementary methods allowed gaining structural knowledge on a number of layered systems: sodium-titanates [6], carbon-silicates [7], CSH phases and hydrotalcites. Here, the successes and pitfalls of the methods will be demonstrated.

[1] Kolb, U., Gorelik, T., Kübel, C., Otten, M.T., Hubert, D. (2007). Ultramicroscopy 107, 507-513. [2] Kolb, U., Gorelik, T.E., Mugnaioli, E., Stewart, A. (2010). Polym. Rev. 50, 385-409. [3] Kolb, U., Mugnaioli, E., Gorelik, T.E. (2011). Cryst. Res. Technol. 46, 542-554. [4] Kolb, U., Mugnaioli, E. (2011) Z. Kristallogr. Proc. 1, 1-13. [5] McCusker, L., Baerlocher, C. (2013). Z. Kristallogr. 228, 1-10. [6] Andrusenko, I., Mugnaioli, E., Gorelik, T.E., Koll, D., Panthöfer, M., Tremel, W., Kolb, U. (2011). Acta Crystallogr. B67, 218-225. [7] Bellussi, G., Montanari, E., Di Paola, E., Millini, R., Carati, A., Rizzo, C., O'Neil Parker, W.J., Gemmi, M., Mugnaioli, E., Kolb, U., Zanardi, S. (2012). Angew. Chem. Int. Ed. 51, 666-669.