3rd Workshop on the Simultaneous Combination of Spectroscopies with X-ray Absorption, Scattering and Diffraction Techniques



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Investigation of crystallization processes using Synchrotron X-ray diffraction and Raman spectroscopy

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The crystallization of polymorphic compounds is investigated in different fields of materials science to understand the stability of materials and their various conversions. The need to control and manipulate the crystallization processes and particularly the final crystal product requires thorough understanding of the underlying crystallization mechanisms and kinetics. This is especially true for drug compounds as the different polymorphs might vary in their physical and chemical properties.

Only in situ characterization methods like X-ray diffraction using synchrotron radiation, enable such detailed investigation of crystallization processes with high time-resolution. By employing an ultrasonic levitator as sample holder the influence of the surface of container walls on the crystallization process can be eliminated. Such setup was used to investigate the crystallization of various organic model compounds. Among those, the compound ROY (5-methyl-2-[(2-nitrophenyl)amino]-3-thiophenecarbonitrile) for which our investigations showed that the resulting crystallization product can be controlled by the choice of the solvent. The combination of synchrotron X-ray diffraction with Raman spectroscopy was used for the characterization of the crystallization process of the organic polymorphic compound nifedipine. Our investigation revealed a strong influence of the solvent on the crystallization mechanism.

Primary author: Ms GNUTZMANN, Tanja (BAM Federal Institute for Materials Research and Testing)

Co-authors: Dr EMMERLING, Franziska (BAM Federal Institute for Materials Research and Testing); Prof. RADEMANN, Klaus (Humboldt-Universitaet zu Berlin, Department of Chemistry); Ms KLIMAKOW, Maria (BAM Federal Institute for Materials Research and Testing)

Presenter: Ms GNUTZMANN, Tanja (BAM Federal Institute for Materials Research and Testing)

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