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Providing datasets to characterize process- or deformation-induced structure formation of polymer materials via in situ synchrotron X-ray experiments

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In this contribution, an overview of experimental results obtained via simultaneous small- and wide-angle X-ray scattering (SWAXS) experiments is given to illustrate its importance in polymer science. Owing to the high spatial and temporal resolution, which can be beyond that of conventional material characterization methods, in situ synchrotron SWAXS experiments are suitable for investigating the structure formation of polymer materials during processing or deformation. For such purposes, the challenge is to develop and provide experimental setups useable for in situ experiments. Such efforts were realized during past long-term projects (LTP) at PETRA III, DESY (Hamburg, Germany). In the case of investigating process- or deformation-induced structure formation of polymer materials, large datasets with a huge amount of information in terms of scattering and metadata are generated. These labeled and well-organized datasets are obtained from various sources, e.g. detectors, motors, sensors etc., and therefore have different data formats, which are (mostly) synchronized. Thus, the achieved datasets are very suitable for polymer material characterization on several length scales –in the range of a few to hundreds of nanometers, e.g. from crystalline to super-molecular structures. By coupling SWAXS with other in situ characterization techniques, such as spectroscopy or digital image correlation, the datasets for material characterization can be further improved, however getting more and more complex. In this context, well-trained and reliable Machine Learning (ML) models could contribute to an even better understanding of the complex material-process-structure-properties relationship for polymers, which can be far beyond current restrictions.

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