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Synthetic polymers: WAXS and SAXS methods to understand materials functionality

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Synthetic polymers can be designed and produced with optimized physical functionalities and find their applications in growing industrial markets such as aerospace, automotive, building products, electronics, energy and medicine. While some of these polymer materials are amorphous, a large proportion exhibit local order with regularly structured domains leading to varying amounts of crystallinity and hence can be characterized by X-Ray diffraction techniques.

Structural information beside phase identification and quantification can be obtained for the polymer crystallinity, the polymer orientation and the crystalline microstructure using wide angle X-ray scattering (WAXS). Additionally, using small angle X-ray scattering (SAXS) techniques also non-crystalline periodicity and domain size distributions can be revealed. Structural variations, such as those induced by e.g. inorganic phases as in composites can be monitored by dynamic studies through in-situ experiments at process conditions (temperature, humidity, mechanical load). Preferred orientation or texturing is a dominant effect in polymers, especially for those obtained by forming procedures such as films processed by solvent casting [1,2] or rigid grid systems produced by 3D printing [3]. Orientation is also the dominant feature in controlling the mechanical and physical properties of polymers which is of major interest for researchers and manufacturers. For the study of those orientation behaviors, a combination of SAXS and WAXS transmission experiments are conducted. Investigations have been made for different synthetic polymer fiber systems.

Polymer-based inks with high cellulose nanocrystal loading are developed for 3D printing of textured cellular architectures. The alignment of CNC particles within the 3D printed filaments leads to enhanced mechanical properties along the printing direction similar to wood and other biological composites [3].

Figure 1 shows X-ray investigations on the 3D printed nano-cellulose system with a strong texturing. The evaluation of the WAXS 2Theta range (partial or complete image integration) reveals information about the crystal structure parameters and the crystallite size of the present cellulose beta polymorph (Fig.1c). In contrast, integrating the azimuth (Fig.1d) gives the possibility to quantify polymer ordering through the evaluation of peak width (FWHM, Herman's parameter). SAXS enables the study of nano-particle size and orientation distributions. The correlation with mechanical properties is drawn and shows the strength of structural understanding for materials system design.

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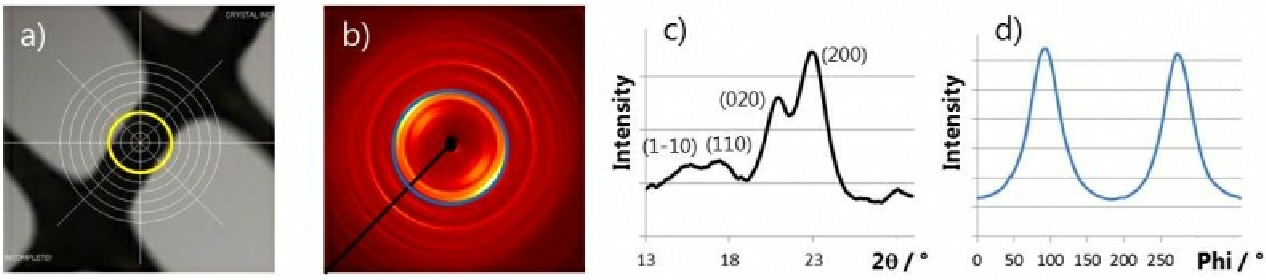

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