Crystal Structure and Texture Refinement of Polymers from Diffraction Images

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The crystal structure of not perfectly crystallized polymers has always been difficult to refine or determine with accuracy especially when a single crystal is not available. Most of them crystallize sufficiently only when strained in fibers. Clearly in this form they are not a single crystal but not even a random powder to permit a reliable crystal structure refinement.

In the present work, we present a methodology to analyze diffraction images of polymers to obtain crystal structure, texture and microstructural information. A laboratory image plate system has been used to collect diffraction images in transmission and reflection diffraction of aligned and strained fibers of different polymers.

The images have been processed in Maud [1] and a structure refinement approach including a Rietveld Texture Analysis [2] was performed for each polymer. An energy approach has been incorporated to help the refinement strategy as well as the use of fragments. From the texture point of view the standard function method for quantitative texture analysis has been developed and successfully applied to these systems. It permits to determine with high accuracy and precision the spread of the single polymers chains in the fibers. The strain applied to the fibers has been modeled by an integrated texture-stress model inside the program as well.

[1] http://www.ing.unitn.it/~luttero/maud [2] Ischia G., Wenk H.-R., Lutterotti L., Berberich F., *J. Appl. Cryst.*, 2005, **38**, 377.

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