APPLICATION NOTE

Polymorphism and crystallite size in β-Polypropylene determined with ARL EQUINOX 100 X-ray diffractometer

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Introduction

Polymer materials are used for a vast number of applications with different demands regarding the resilience of the material. One of the most common materials is Polypropylene (PP) because of its cost efficiency and availability. The mechanical and chemical resilience of polymer materials not only depend on type and crystallinity but also on the polymorphic structure and domain size (crystallite size, CS). Using β-PP instead of α-PP clearly increases both chemical resilience and impact strength while the viscosity remains comparable to α-PP.

Instrument

The Thermo Scientific™ ARL™ EQUINOX 100 X-ray diffractometer employs a custom-designed Cu (50 W) or Co (15 W) micro-focus tube with mirror optics. Such a low wattage system does not require external water chiller or other peripheral infrastructure, allowing the instrument to be easily transported from the laboratory to the field or between laboratories.

**Figure 1:** ARL EQUINOX 100 X-ray diffractometer.

The ARL EQUINOX 100 (c.f. Figure 1) provides very fast data collection times compared to other conventional diffractometers thanks to its unique curved position sensitive detector (CPS) that measures all diffraction peaks simultaneously and in real time. It is therefore well suited for both reflection and transmission measurements.

For XRD measurements, a sheet sample PP (Polypropylene) was measured in transmission geometry for 5 min under Cu-Kα radiation. The quality of the data obtained with benchtop ARL EQUINOX 100 is comparable to data from a typical high-power floor standing instrument. Qualitative analysis was carried out using MDI JADE 2010 with the ICDD PDF4+ Organic database. CS was determined using Le Bail fitting and Scherrer's equation.

Results

Comparing the data to ICDD PDF4+ Organic database clearly yields predominantly β-PP (blue) and traces of α-PP (grey) as results, whereas the domain sizes differ between β-PP (33 nm) and α-PP (10 nm). (c.f. Figure 2)

Figure 2: Diffraction pattern of β-PP (blue) and α-PP (grey).
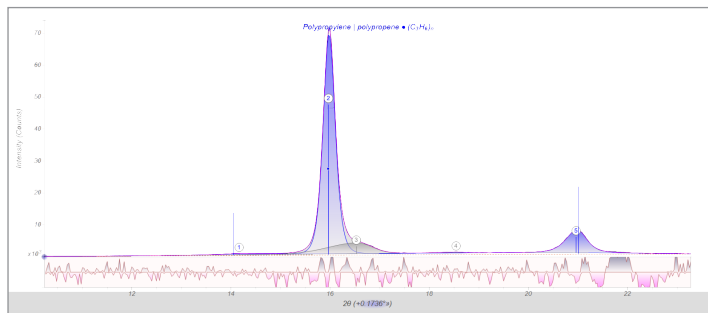
Conclusion

The ARL EQUINOX 100 benchtop XRD instrument in combination with the MDI JADE 2010 software suite and ICDD pdf4+ Organic database is a quick screening solution to conveniently determine the crystallite size and polymorphism of polymer materials. The intergrowth structure of α- and β- PP is crucial for the properties of the resulting material which is widely used in industrial applications.

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