Chemical Microstructure of Copolymers

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For copolymers both the molecular weight distribution (MWD) and chemical composition distribution (CCD) have important effects on the physical properties of polymers. While the MWD is routinely determined using chromatography, the CCD cannot be determined directly by use any existing experimental technique.

Temperature-rising elution fractionation (TREF) is widely used to estimate the CCD of semi-crystalline copolymers by relating the elution temperature to the average comonomer content. However, this experimental technique is very laborious. Recently a new technique called crystallization analysis fractionation (CRYSTAF) has been developed based on the single-step crystallization of polymers in solution. Providing comparable information to TREF, CRYSTAF requires much less analysis time. Like TREF, CRYSTAF data do not lead directly to the CCD, and a calibration curve is required that relates the crystallization temperature to the average comonomer content.

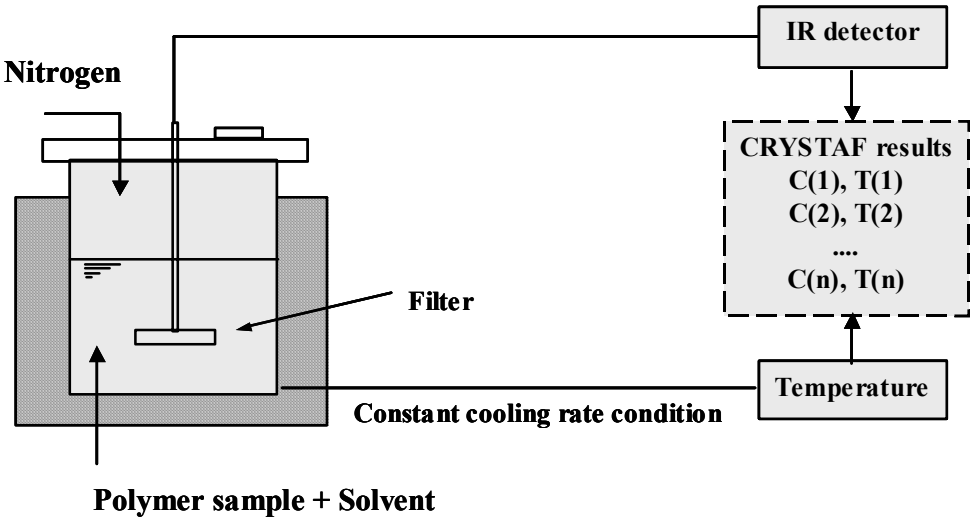

Figure 1. Schematic diagram of CRYSTAF analysis

The main objective of this study is to develop a technique to determine the CCD by (1) modeling the fractionation process in CRYSTAF, and (2) constructing the relationship between the CRYSTAF profile and the CCD. Monte Carlo simulation will be used to generate microstructural information for the study of the fractionation process. Both TREF and CRYSTAF experiments will be performed to determine the mechanism of crystallization.

While a theory for CCD in binary copolymers has been developed by Stockmayer, there is no appropriate theory describing CCD in multi-component copolymers. Another objective of the present study then is to develop a theory for describing the CCD in a multi-component system using a statistical approach.