529d The Application of Cluster Size Distribution Methods in Polymer Crystallization Kinetics

Jiao Yang, Benjamin J. McCoy, and Giridhar Madras

Cluster size distribution (CSD) kinetics is adopted to explore the kinetics of polymer crystallization. Population balance equations based on crystal size distribution and concentration of amorphous polymer segments are solved numerically and the related dynamic moment equations are also solved. The model accounts for heterogeneous or homogeneous nucleation and crystal growth. Homogeneous nucleation rates follow the classical surface-energy nucleation theory. Different mass dependences of growth and dissociation rate coefficients are proposed to investigate the fundamental features of nucleation and crystal growth. We also investigate the effect of temperature on homogeneous nucleation and crystal growth for isothermal polymer crystallization. The model includes the temperature effects of interfacial energy, nucleation rate, growth and dissociation rate coefficients, and equilibrium solubility. The time dependencies of polymer concentration, number and size of crystals, and crystallinity (in Avrami plots) are presented for different temperatures. The denucleation (Ostwald ripening effect) is investigated by comparing moment and numerical solutions of the population balance equations. The application of the CSD model is also extended to nonisothermal condition. The time dependencies of polymer concentration, number and size of crystals, and crystallinity (in Avrami plots) are presented for different cooling rates. The incubation period is also investigated at different cooling rates and different initial temperatures. The relationship between cooling rates and incubation time is presented graphically and compared with experimental measurements. The initial temperature (relative to melting point) has a significant effect on nonisothermal crystallization. A comparison of moment and numerical solutions of the population balance equations shows the influence of Ostwald ripening. Agreement between modeling results and experimental measurements at different cooling rates supports the application of the distribution kinetics model for polymer crystallization.