Saraporn Ketdee 2007: Simulation of Morphological Development during Isothermal Crystallization of Polymers. Master of Engineering (Chemical Engineering), Major Field: Chemical Engineering, Department of Chemical Engineering. Thesis Advisor: Assistant Professor Siripon Anantawaraskul, Ph.D. 73 pages.

The effect of number of predetermined nuclei, growth rate, and crystallization temperature on crystallization kinetics and detailed morphological development during isothermal crystallization of polymer was investigated using a stochastic simulation.

The results show that number of predetermined nuclei significantly affects both crystallization kinetics and polymer morphology. An increase in the number of predetermined nuclei fastens a crystallization process by speeding up the impingement phenomena and increasing the levels of impingement. A growth rate has a stronger impact on crystallization kinetics, but it only helps speed up the impingement phenomena without increasing the level of impingement. Although a growth rate influences an average spherulite size and distribution of spherulite size during the crystallization, it has no effect on a final morphology.

The crystallization temperature significantly affects both crystallization kinetics and polymer morphology, as it strongly influences the number of predetermined nuclei and spherulite growth rate. In this work, poly (trimethylene terephthalate) is used as a reference material. When crystallization temperature is higher than 70^{o}C, both number of predetermined nuclei and spherulite growth rate increase with crystallization temperature. Therefore, crystallization is completed faster as crystallization temperature decreases. The competing effect of number of predetermined nuclei and spherulite growth rate occur in crystallization temperature range of $40^{0}\,\mathrm{C} \le T_{c} \le 70^{0}\,\mathrm{C}$. The results show that at crystallization temperature range from 60^{o}C to 70^{o}C, the kinetic of crystallization process is mainly governed by the effect of number of predetermined nuclei. However, at the temperature lower than 60^{o}C, the kinetics of crystallization process is mainly controlled by the effect of growth rate.

The quantitative understanding on morphological development obtained from this work will be the key element for further constructing quantitative morphology-property relationships.

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