SIMULATION OF MORPHOLOGICAL DEVELOPMENT DURING ISOTHERMAL CYRYSTALLIZATION OF POLYMERS

INTRODUCTION

Polymers have been widely used for many applications in our daily life. Many kinds of equipment and construction material are made from polymer, for example, house wares, grocery bags, shampoo bottles, children's toys science equipments, and medical equipments**.** This versatile material also has advantages of having low weight, cheap, and easy to form into a preferred shape.

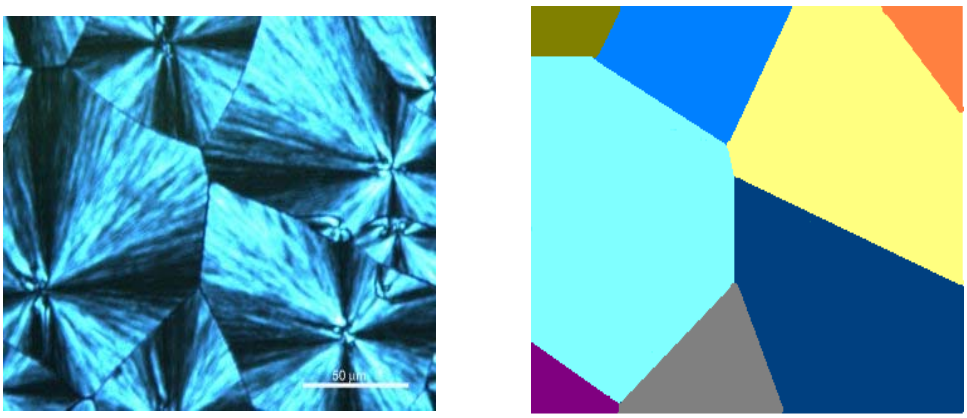
The polymer is generally produced commercially in pellet form before transforming into many useful things. To form polymer article, several processing techniques have been used. The typical steps involved are melting the polymer resin, forming to a desired shape, and solidification. The solidification, or crystallization, step usually held the key to physically modify the article properties.

For several semi-crystalline polymers, the polymer crystals formed during the crystallization step are in form of spherulite. As the crystallization step proceeds, the spherulites grow until they fill all the possible spaces. The spherulite filled region is called crystalline phase, and the other region called amorphous phase. Percent crystallinity (percent of filled space) and both average and distribution of spherulites can be influenced by operating condition (e.g., temperature, pressure, and shear stress) and, thus, can be modified to a certain degree. This polymer morphology determines the physical properties. Therefore, it is of interests for polymer engineer.

To experimentally examine the spherulites growth process during the crystallization step, the polarized light microscope (PLM) and atomic force microscope are typically used. However, the experimental approach has a drawback that it can not provide quantitative morphological details.

Recently, there are several attempts to model this growth process and obtain the final morphology because the modeling approach has an advantage of being able to separately examine each crystallization parameter (e.g., growth rate, variation of growth rates, number of predetermined nuclei, mode of nucleation, and rate of nucleation), providing some new insights on the processing improvement. This can not be done in the experiment as several phenomena occurred simultaneously. Furthermore, the modeling approach can extend the domain to gather the information on distribution of spherulite size, which is extremely difficult, if possible at all, to achieve. The information of the distribution of spherulite size could be used to construct the morphology-properties relationships.

Previously proposed models help provide insights on the final morphology, but none investigates the morphological development in details. In this work, we implement the Monte Carlo simulation to probe the effect of crystallization parameters (e.g., crystallization temperature, number of predetermined nuclei and growth rate) on morphological development (e.g., crystallinity, average crystalline size, and distribution of crystalline as a function of time) during isothermal crystallization of polymer. Under this condition, the heterogeneous nucleation (i.e., nuclei occurred randomly in space at the same time) and constant growth rate are assumed. In our model, the crystallite is considered in a form of spherulite, which is a typical shape of polymer crystalline.



(a) (b)

Figure 1 Comparison between the final morphology obtained from (a) polarized light microscope (PLM) and (b) simulation

Objective

The objective of this work is to study the effect of crystallization parameters (e.g., crystallization temperature, number of predetermined nuclei and growth rate) on crystallization kinetics and morphological development (e.g., crystallinity, average crystalline size, and distribution of crystalline as a function of time) during isothermal crystallization of polymers.

Scope of Thesis

In this work, the morphological developments of spherulites under various isothermal conditions were investigated in a square lattice with 800x800 meshes using a model based on a Monte Carlo simulation. Particularly, the effects of growth rate, number of predetermined nuclei, and crystallization temperature in the range of 40^{o}C-90^{o}C on the crystallinity, average crystallite size, and size distribution at various time steps were studied in great details.