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Spherulite Microstructure Formation Simulation Based on Effect of Molding Conditions on Polylactic Acid

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Thermoplastic polymers are increasingly being used in a wide range of fields because of their light weight, low cost and excellent formability. Crystalline polymers, which means thermoplastic polymers with semicrystalline phase, have a mixture of a crystalline phase with a stable folding structure of molecular chains and an amorphous phase with a disordered structure on a microscopic scale. These two layers are alternately stacked to form a structure: lamellar crystal. In addition, it is known that lamellar crystals grow radially to produce a crystalline structure, which is called a spherulite. The mechanical properties of crystalline polymers are closely related to the dimensions of the spherulite and the crystallinity, and the morphology of spherulite depends on the molding conditions such as temperature and pressure.

Evaluation of the effect of the spherulite microstructure on the mechanical properties of crystalline polymers can improve the accuracy of structural analysis. Various studies have been conducted on microstructure and crystallization models. However, since the spherulite is a complicated structure composed of amorphous and crystalline phases, the effects of actual molding conditions on spherulite microstructure formation and changes in mechanical properties depending on spherulite microstructure remain to be clarified.

This study investigates a simulation model predicting spherulite microstructure formation based on experimental observations. The crystallization process of polylactic acid is observed at different molding temperatures by in-situ observation, and the rate of spherulite formation and growth is estimated. Furthermore, according to the Turnbull-Fisher primary nucleation model and the Lauritzen-Hoffman secondary nucleation model, Monte Carlo simulations of spherulite microstructure formation are performed based on the obtained experimental results. The validity of the method is verified by a comparison of the simulated and the experimental results.