결정화거동을 고려한 신장변형공정의 안정성 분석

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Stability Analysis of Extensional Deformation Processes with Crystallization Kinetics

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Introduction

Crystallization kinetics is an important phenomenon for extensional deformation processes. To describe the crystallization kinetics (Fig. 1), thermally-induced and flow-induced crystallization kinetics have been proposed for extensional deformation processes [1-6]. Thermally-induced crystallization of polymer processing have been well understood. Experimentally-observed thermally-induced crystallization can be reproduced by empirical relation [1]. In the extensional deformation processes, not only thermally-induced crystallization but also flow-induced crystallization is important to clearly analyze the process, especially high-speed fiber spinning process. Flow-induced crystallization, however, make the system more difficult to be analyzed due to its high nonlinearity. Ziabicki [1] used the exponential function type equation based on thermodynamics to represent flow-induced crystallization kinetics of fiber spinning process. And many researchers in succession [2,3] reported excellent simulation results with flow-induced crystallization. On the other hand, Jaydeep and Beris [4,5] divided polymer system into amorphous and crystalline phases. To model each phase, they used extended White-Metzner model for amorphous phase and Leonov model with infinite relaxation time for crystalline phase. Recently, Doufas and McHugh [6] introduced micro-structural model before and after the onset of crystallization, respectively. In the amorphous phase, modified Giesekus model was used to describe stretchable polymer chain, while rigid rods model was used to represent the orientation and growth at the expense of flexible portions of the chains for semi-crystalline phase.

In this paper, using the crystallization models, the stability of extensional deformation processes like fiber spinning and film casting process is determined by transfer function approach based on frequency response and transient response on the step disturbance.

Modeling

To describe fiber spinning process with crystallization kinetics (Fig. 2), Ziabicki's model is adopted to analyze the extensional deformation processes. The dimensionless governing equations of fiber spinning process with flow-induced crystallization are presented as shown below.

Equation of continuity: $$\frac{\partial a}{\partial t} + \frac{\partial (av)}{\partial z} = 0 \qquad (1)$$

where, $a=\frac{A}{A_0}$, $v=\frac{V}{V_0}$, $t=\frac{t' V_0}{L}$, $z=\frac{Z}{L}$

Equation of motion:

$$C_{in}\left(\frac{\partial v}{\partial t}+v\frac{\partial v}{\partial z}\right)=\frac{1}{a}\frac{\partial(a\tau)}{\partial z} \qquad (2)$$

where, $C_{in}=\frac{\rho V_0 L}{2\eta_0}$, $\tau=\frac{\tau' L}{2\eta_0 V_0}$

Constitutive equations (Phan-Thien-Tanner model):

$$K\tau+De\left[\frac{\partial\tau}{\partial t}+v\frac{\partial\tau}{\partial z}-2(1-\xi)\tau\frac{\partial v}{\partial z}\right]=\frac{De}{De_0}\frac{\partial v}{\partial z} \qquad (3)$$

where, $K=\exp[2\varepsilon De_0\tau]$, $De_0=\frac{\lambda_0 V_0}{L}$, $De=De_0\exp\left[k\left(\frac{1}{\theta}-1\right)\right]$

Equation of energy:

$$\frac{\partial\theta}{\partial t}+v\frac{\partial\theta}{\partial z}=\mathrm{St}\,v^{1/3}a^{-5/6}(\theta_a-\theta)\left[1+\left(8\frac{v_y}{v}\right)^2\right]^{1/6}+\frac{\triangle H_c}{C_p}\left(\frac{\partial x}{\partial t}+v\frac{\partial x}{\partial z}\right) \qquad (4)$$

where, $\theta=\frac{T}{T_0}$, $x=\frac{X}{X_{eq}}$, $\mathrm{St}=\frac{1.67\times10^{-4}L}{\rho C_p A_0^{5/6}V_0^{2/3}}$

Equation of crystallization:

$$\frac{\partial x}{\partial t}+v\frac{\partial x}{\partial z}=(1-x)nK_{\max}\exp\left[-4\ln2\frac{(\theta-\theta_{\max})^2}{d^2}+Cf_a^2\right]\left[\ln\left(\frac{1}{1-x}\right)\right]^{\frac{n-1}{n}} \qquad (5)$$

Birefringence:

$$\varDelta n=(1-x)f_a\varDelta a^0+xf_c\varDelta c^0 \qquad (6)$$

Boundary conditions:

t=0: $a=a_s,\ v=v_s,\ \tau=\tau_s,\ \theta=\theta_s,\ x=x_s$ for $0<z<1$

t>0: $a=a_0=1,\ v=v_0=1,\ \theta=\theta_0=1,\ x=x_0=0$ at z=0

$v=v_L=r(1+\varepsilon^*)$ at z=1

where, a is the dimensionless spinline cross-sectional area, v is the dimensionless spinline velocity, τ is the dimensionless stress, θ is dimensionless temperature, x is dimensionless crystallinity, t is dimensionless time, θ_a is ambient temperature, v_y is cooling air velocity, C is the enhancement of crystallization rate due to orientation, f_a and f_c is orientation factor of amorphous and crystalline phases, $\varDelta a^0$ and $\varDelta c^0$ are birefringence factor of amorphous and crystalline phases, *De* is Deborah number, *St* is Stanton number, ε and ξ are PTT model parameters, *r* is drawdown ratio, ε^* is constant representing the initial disturbance at the take-up, and subscript *0*, *L*, *S* denote spinnert, take-up, and steady state condition, respectively.

Results

Though the governing equations represent for fiber spinning process, the film casting process, one of the extensional deformation processes, can be simulated by similar method. The effects of crystallization on the stability are determined by the transfer function approach, which was introduced by Kase's group [7,8] for fiber spinning process. In this method, the stability is determined by Bode' diagram with frequency change. As crystallization kinetics constant is increased, the crystallization rises and film casting process is stabilized for both extension thickening and extension thinning fluids (Fig. 3). It has been found that thermally-induced crystallization is mainly affected to the film casting process under the industrial operating conditions by the Ziabicki's model. That is, the flow-induced crystallization has a minor effect on the dynamics of a system. To clearly confirm the effects of flow-induced crystallization on the process stability, higher extrusion and take-up speed conditions than usual process conditions are required.

Therefore, high-speed spinning is a typical process to represent flow-induced crystallization. As shown in Fig. 4, the steady state profile is made to jut out at a right angle because of flow-induced crystallization, when the take-up velocity is larger than 6000m/min. As the extrusion velocity increases, the position to occur flow-induced crystallization becomes more distance from the take-up. The further details of flow-induced crystallization on the process stability will be reported on the presentation.

Acknowledgements

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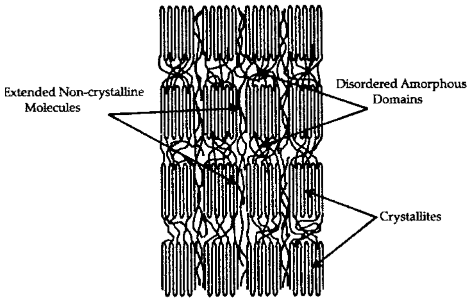


Figure 1. Schematic representation of the semi-crystalline polymer for the Flory model.

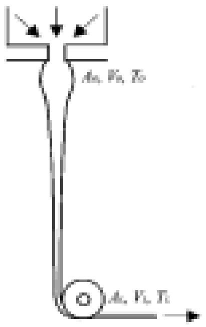
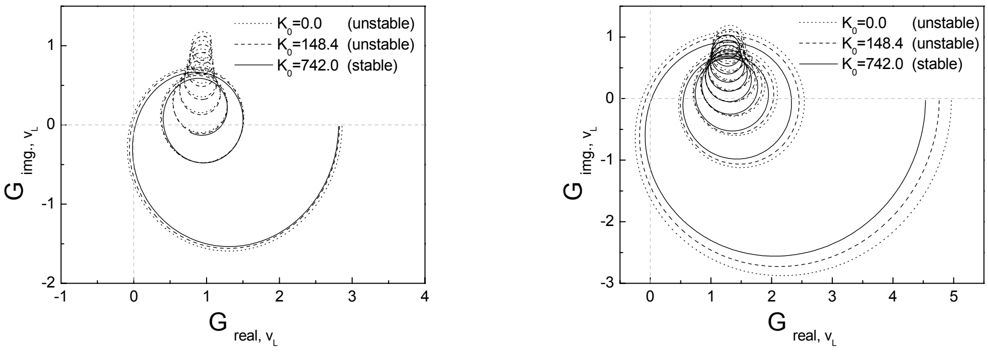
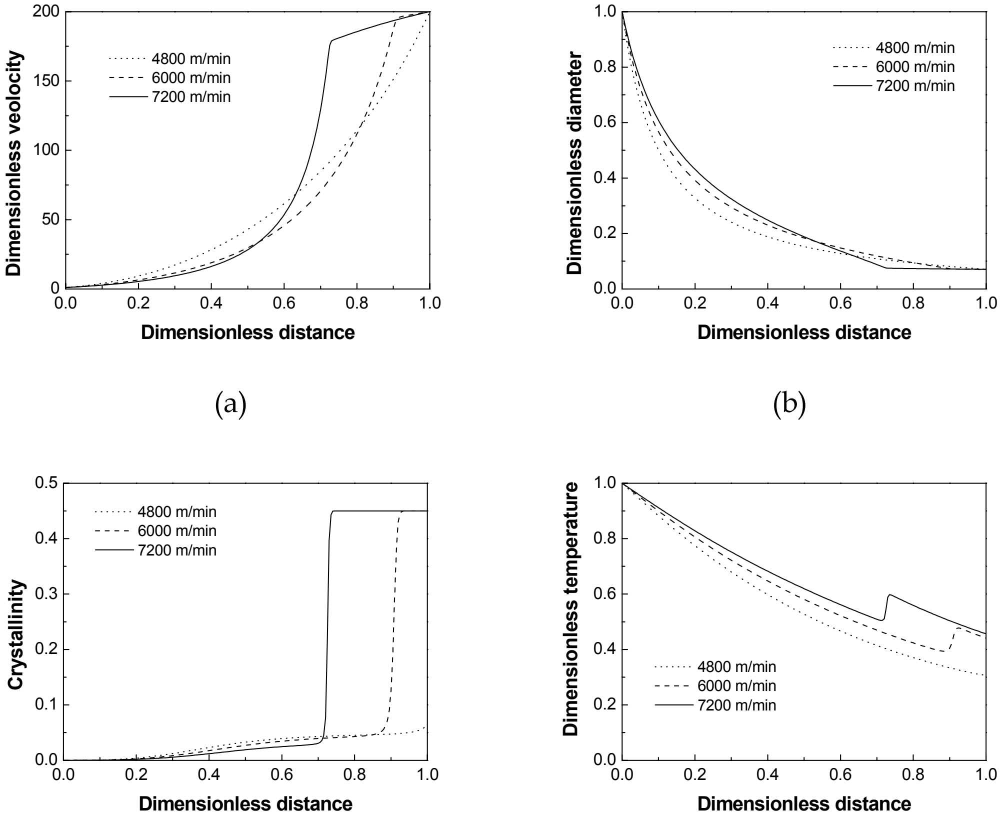


Figure 2. Schematic diagram of fiber spinning process



(a) (b)

Figure 3. Transfer function approaches to determine process stability of the film casting process for (a) extension thickening and (b) extension thinning fluids



(a) (b)

(c) (d)

Figure 4. Effect of take-up speed at the same draw ratio on the (a) velocity profile, (b) dimensionless diameter, (c) crystallinity and (d) dimensionless temperature of fiber spinning process using Ziabicki's model.