

# Structure development during solidification in the processing of crystalline polymers

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# Structure Development During Solidification in the Processing of Crystalline Polymers

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## Introduction

During processing of thermoplastic crystalline polymers, the solidification conditions are very drastic. Knowledge of material behaviour assessed through standard equipment is restricted to very narrow temperature, time and deformation rate ranges. In particular this holds for its structure development. From the technological point of view the morphology of the solidified product and the molecular composition are the main determining factors of the mechanical properties.

## **Objectives**

- investigate the mechanisms of solidification of semicrystalline thermoplastic polymers.
- development of a numerical model for the crystallisation under flow of semicrystalline polymers.

# Theory



## fig. 1 A crystalline structure

For a semi-crystalline polymer it is impossible to reach full crystallinity, because of the long molecular chains. An amorphous region is present between the crystals (fig.1). In the crystals crystalline regions are present as the spokes of a wheel.

## Modelling

A model used to calculate the degree of crystallinity  $\xi_g$  is [1]:

$$\dot{\xi}_g = G(t)\phi_1(t)e^{-\phi_0(t)}$$
$$\phi_i(t) = G(t)^{-1}\dot{\phi}_{i-1}$$
$$\dot{\phi}_3(t) = 8\pi\alpha(t)$$

As an example, for a strip the temperature and degree of crystallinity are given (fig.2 and 3):



**fig. 2** *Temperature as a function of time in the thickness for different points (0-4 sec.:filling stage).* 



**fig. 3** The degree of crystallinity as a function of time.

## **Experimental**

An experimental setup is developed to measure the specific volume as a function of pressure, temperature, volume and cooling rate (fig.4). In this way the degree of crystallinity can be calculated:

 $\xi_g.\rho_{crystal} + (1 - \xi_g).\rho_{amorph.} = \rho_{meas.}$ 



fig. 4 The experimental setup

## **Materials involved**

- □ Stamylan HDPE by DSM,
- Daplen PP by PCD Polymere,
- □ PB by Shell,
- □ PET by Sinco Engineering.

# **Discussion**

For a realistic description of the crystallisation process, advanced theoretical models and experiments are combined. Results will be implemented in the numerical tool VIp.

### **References:**

[1] SCHNEIDER ET AL.: Non-isothermal Crystallisation, Crystallisation of Polymers (System of Rate Equations) (Intern. Pol. Proc. II (1988) 3/4, 151-154).