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Introduction

Elastic moduli of semi-crystalline polymers are important properties and difficult to predict due to their dependence on many factors, such as: molecular weight, cooling rate, annealing, etc. To better design products, it is of significance to accurately predict these properties as a function of the microstructural morphology and crystallinity.

Micromechanical Model

Semi-crystalline polymers can be modeled as two-phase composites, the crystalline phase and the amorphous phase. By using a layered micromechanical model, overall properties can be predicted as a function of crystallinity (figure 1).

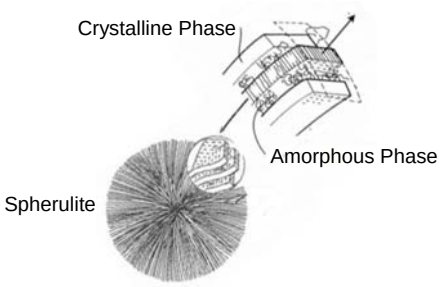

Figure 1: Morphology of a spherulitic semi-crystalline polymer [1].

It is shown that a three-phase model can better predict the elastic modulus of semi-crystalline polymers [2], as a two phase model ignores the effect of the inter-phase, which has properties between the crystalline and amorphous phases.

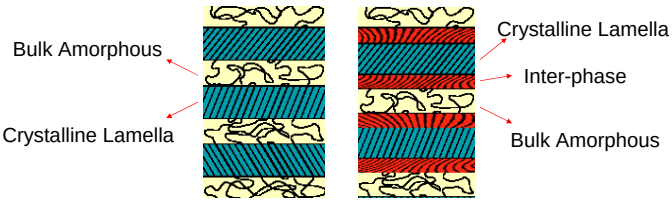

Figure 2: Schematic of the two-phase and three-phase models

Interface conditions:

$$\begin{cases} \boldsymbol{\sigma}^a \cdot \vec{n} = \boldsymbol{\sigma}^c \cdot \vec{n} = \boldsymbol{\sigma}^I \cdot \vec{n} \\ \vec{x}_i \cdot \boldsymbol{\varepsilon}^a \cdot \vec{x}_j = \vec{x}_i \cdot \boldsymbol{\varepsilon}^c \cdot \vec{x}_j = \vec{x}_i \cdot \boldsymbol{\varepsilon}^I \cdot \vec{x}_j \end{cases}$$

The three-phase model also incorporates crystalline lamellar and inter-phase thicknesses, while no length scales were included in the two-phase model.

Homogenization Methods

Three methods have been used for obtaining the overall properties: Voigt, Reuss and Voigt-Reuss-Hill average.

Results and Discussion

In this section, a two-phase and a three-phase composite inclusion model are used to obtain the effective behavior of HDPE. The spherulitic structure of HDPE is presented by an aggregate of 120 inclusions with random orientation of crystallographic directions and interface normals (figure 3). Monte-Carlo simulation results show that δ^r =1 to 2 nm (inter-phase thickness) while δ^c =6.8 nm (crystal thickness) [2].

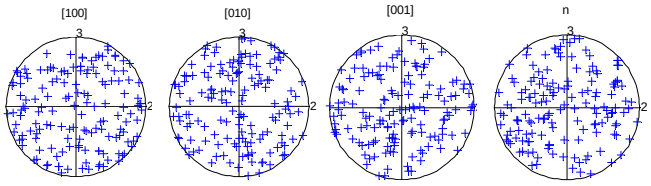

Figure 3: Equal area projection pole figures of random orientation of crystallographic directions and interface normals

It can be seen in figure 4 that a three-phase model agrees much better with experiments than a two phase model.

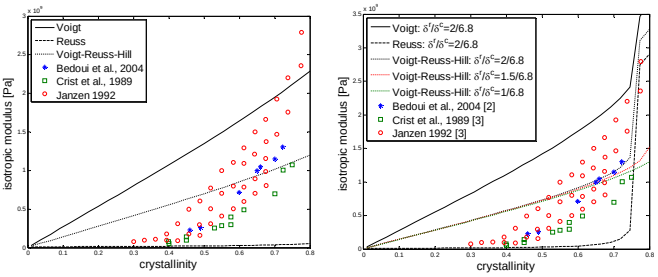

Figure 4: Predicted Young's modulus using a two-phase model (left) and a three-phase model with different inter-phase thickness (right).

Conclusions and Future Work

✓ The properties of semi-crystalline polymers can better be predicted if a three-phase composite inclusion model is used.

✓ Hybrid interaction models will be used to form an intermediate approach between the upper bound Voigt and the lower bound Reuss models.

References

[1] L. Lin, A.S. Argon, Journal of Materials Science, 29 (1994): 294-323

[2] T.N. Pham, C.L. Tucker, Polymer processing society 24th annual meeting, 2008, Italy

[3] X. Guan, R. Pitchumani, Polymer Engineering and Science, 44(3) (2004): 433-451.