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Massachusetts Institute
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SIMULATION OF DEFORMATION AND EVOLUTION IN SEMI-CRYSTALLINE POLYMERS

S. Ahsi, D. Parks, and A. Argon

Department of Mechanical Engineering
Massachusetts Institute of Technology
Cambridge, MA 02139

INTRODUCTION

We developed a spectrum of mechanically-based models [1,2] (constrained hybrid model and a composite model) which can be applied to the study of deformation and texture evolution in semi-crystalline polymers. We applied these models to predict the behavior and texture at large deformations, and we compared our predictions to experimental data. The agreement with the experiments is satisfactory.

MODELLING

Our major assumptions are that the elasticity is entirely neglected and the plasticity is incompressible and time dependent. The crystalline phase deforms by slip on crystallographic planes and directions and the amorphous phase deformation can be modelled by an isotropic linear or non-linear viscous material.

The composite model is based on the resolution of a composite inclusion problem. The composite inclusion (lamella and amorphous layer) is submitted to a strain rate $\underline{D}^I$. This local strain rate depends on the macroscopic strain rate $\underline{D}$ (applied to the matrix) and on the constraint due to the non-extension of the lamella in chain direction. The constrain implies the lack of five independent systems in the crystalline phase and therefore the non-applicability of the classical Taylor model (uniform deformation) to the crystalline phase.

2.1 Crystalline phase behavior

Because of inextensibility in chain direction, the strain rate $\underline{D}^I$ within the crystalline domain should have a zero projection in chain direction:

$$\text{or } \underline{\epsilon} \cdot \underline{D}^I \cdot \underline{\epsilon} = 0 \quad (1a)$$

$$\underline{C} \cdot \underline{D}^I = \underline{C}' \cdot \underline{D}^I = 0 \quad (1b)$$

$$\text{where } C_{ij} = c_i c_j, \quad (2)$$

$\underline{C}'$ is the deviatoric part of $\underline{C}$, and c is a crystallographic vector in chain direction.

The deviatoric Cauchy stress $\underline{S}^I$ within the crystalline domain can be decomposed as follows:

$$\underline{S}^I = \underline{S}^{I*} + S \underline{C}' \quad (3)$$

$\underline{S}^{I*}$ is the stress part producing the strain rate $\underline{D}^I$ and S is an arbitrary crystalline stress component in the constraint "direction" (chain direction).

The constitutive law for the crystalline domain (lamella) is given by the following non-linear relation [3]:

$$\frac{\underline{D}^I}{\dot{\gamma}_0} = \sum_s \underline{R}^s \left(\frac{\underline{R}^s \cdot \underline{S}^{I*}}{r_c^s} \right)^n \quad (4)$$

where $\dot{\gamma}_0$ is a microscopic reference strain rate, r_c^s is the critical resolved shear stress and $\underline{R}^s$ is the symmetrical part of the Schmid tensor for the slip system s . The summation in (4) extends over all active slip systems.

2.2 Amorphous phase behavior:

The amorphous domain behavior can be represented by the following relation

$$\underline{D}^a = F(\underline{S}^a, \dots) \quad (5)$$

where $\underline{S}^a$ and $\underline{D}^a$ are the deviatoric Cauchy stress and the strain rate within the amorphous layer, respectively. A special case of (5) is the following non-linear relation:

$$\underline{S}^a = \mu (\underline{D}^a)^{m_a - 1} \underline{D}^a \quad (6)$$

where μ and m_a are material constants. If m_a is set equal to 1, then the amorphous phase is simply assumed to be linear viscous, a crude model of amorphous behavior above T_g .

Other models of the amorphous phase behavior [4] can also be represented by equation (5).

2.3 Composite Behavior (lamella and amorphous layer)

The composite inclusion (fig. 1) is made of a lamella and an amorphous layer. The crystallographic axis $\underline{\epsilon}$ in chain direction can either be parallel to the lamella normal $\underline{n}$ or not.

When $\underline{\epsilon}$ is not parallel to $\underline{n}$, then an arbitrary inclusion average strain rate component in the $\underline{C}'$ direction can be accommodated by the amorphous phase deformation. If $\underline{\epsilon}$ and $\underline{n}$ are parallel, the inclusion strain rate $\underline{D}^I$ is constrained:

$$\underline{C}' \cdot \underline{D}^I = 0 \quad (7)$$

Here, we assume the latter case and we assume further that $\underline{n}$ and $\underline{\epsilon}$ remain parallel with ongoing deformation (clearly these are drastic simplifications and more general models are under development [2]).

Each inclusion I (fig. 1) should deform in a way to preserve compatibility and equilibrium at its internal lamella amorphous interface. These conditions imply continuity of some stress and strain rate components; the other components are related by the mixture law:

$$\underline{D}^I = f_a \underline{D}^a + (1 - f_a) \underline{D}^I \quad (8)$$

$$\begin{aligned}\underline{S}' &= f_a \underline{S}^* + (1 - f_a) \underline{S}^* \\ &= f_a \underline{S}^* + (1 - f_a) (\underline{S}^{*,c} + S \underline{C}')\end{aligned}\quad (9)$$

f_a is the volume fraction of the amorphous phase.

The missing stress component S is assumed to be equal to the macroscopic corresponding stress component,

$$S = \left(\frac{3}{2} \underline{S} \cdot \underline{C}' \right) / (1 - f_a) \quad (10)$$

$\underline{D}'$ is given by the constrained Hybrid model [1], by using local compatibility and equilibrium conditions at the interface and equations (8), we can solve for $\underline{D}^*$ and $\underline{D}^c$. We can then derive the stresses from the constitutive equations of crystalline and amorphous phases. The macroscopic stress is obtained from an averaging consistency condition.

RESULTS

We applied the composite model to predict behavior and texture evolution in polyethylene (70% crystallinity) in an initially isotropic (quasi spherulitic) condition. Figure 2 shows the stress strain curve for tension in comparison with G'Sell and Jonas's [5] data. Figure 3 shows the pole figures (002) and (200) after 175% tension. We can see that we predict a fiber texture with c axis parallel to the tension direction.

It is shown in figures 2-3 that our predictions are in good agreement with experiments.

Results from an idealized 100% crystalline model [1] showed a similar texture evolution, but equivalent sharpness textures were obtained at considerably smaller tensile strains. This indicates that a primary role of the amorphous material is to provide additional straining without substantial effect on crystallographic texture.

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REFERENCES

1. D.M. Parks and S. Ahsai (To be published).
2. D.M. Parks and S. Ahsai (To be published).
3. J.W. Hutchinson, *Proc. Roy. Soc.*, **A348**, 101, (1976).
4. M.C. Boyce, D.M. Parks, and A.S. Argon, *Mech. of Mat.*, **7**, 15, (1988).
5. C. G'Sell and J.J. Jonas, *J. of Mat. Sci.*, **14**, 583, (1979).

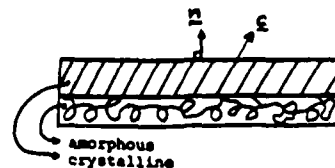


fig. 1: composite inclusion.

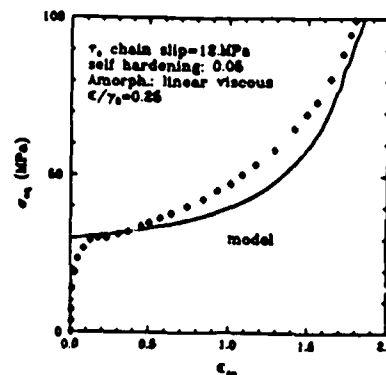


fig. 2: stress-strain curve for tension test in comparison with G'Sell & Jonas's data.

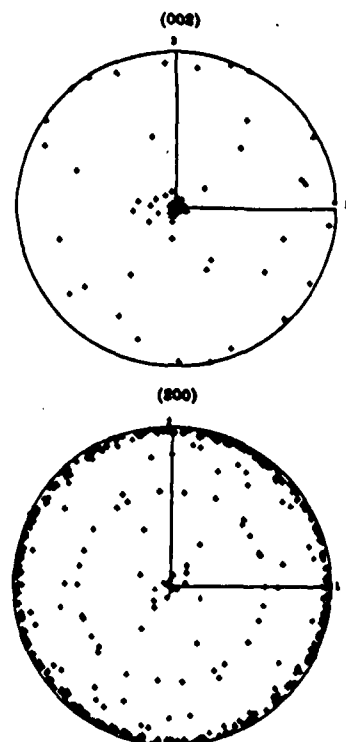


fig. 3: (002) & (200) pole figures after 175% tension (axe 3 = tension direction).