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Self-consistent modeling of large plastic deformation, texture and morphology evolution in semi-crystalline polymers

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Abstract

A self-consistent model for semi-crystalline polymers is proposed to study their constitutive behavior, texture and morphology evolution during large plastic deformation. The material is considered as an aggregate of composite inclusions, each representing a stack of crystalline lamellae with their adjacent amorphous layers. The deformation within the inclusions is volume-averaged over the phases. The interlamellar shear is modeled as an additional slip system with a slip direction depending on the inclusion's stress. Hardening of the amorphous phase due to molecular orientation and, eventually, coarse slip, is introduced via Arruda–Boyce hardening law for the corresponding plastic resistance. The morphology evolution is accounted for through the change of shape of the inclusions under the applied deformation gradient. The overall behavior is obtained via a viscoplastic tangent self-consistent scheme. The model is applied to high density polyethylene (HDPE). The stress–strain response, texture and morphology changes are simulated under different modes of straining and compared to experimental data as well as to the predictions of other models.

Keywords: Micromechanics; Constitutive behavior; Polymer; Self-consistent; Texture

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1. Introduction

Semi-crystalline polymers are increasingly used in structural applications where the influence of the microstructure and its evolution on the macroscopic mechanical properties is of prime importance. A number of applications, such as thin films, coatings, high-modulus fibers and ribbons, display highly anisotropic mechanical and crystallographic properties and their processing often involves large plastic deformation of an initially isotropic material.

The microstructure of melt-crystallized polymers consists of broad, thin crystalline lamellae separated by amorphous layers. Locally, the lamellae are grown from a central nucleus and are radially oriented, which results in the formation of spherulitic structures (e.g. Lin and Argon, 1994). During large plastic deformation, profound changes in both the crystallographic texture and morphology take place. It has been observed (e.g. Butler et al., 1998; Hiss et al., 1999) that in uniaxial tension of HDPE, the initial lamellar microstructure is gradually destroyed and replaced by stretched fibrils (Fig. 1). Similar lamellar-to-fibrillar transition processes have also been reported from simple-shear experiments of HDPE (Bartczak et al., 1994).

In the past fifteen years, several micromechanical models have been developed in order to simulate the stress–strain behavior and crystallographic texture evolution in semi-crystalline polymers at large strains. Parks and Ahzi (1990) proposed a purely crystalline model treating the lack of five independent slip systems in polymer crystals. Ahzi et al. (1990) developed a bi-crystal approach, where the basic structural unit of semi-crystalline polymers was introduced as a two-phase composite inclusion consisting of a single, flat

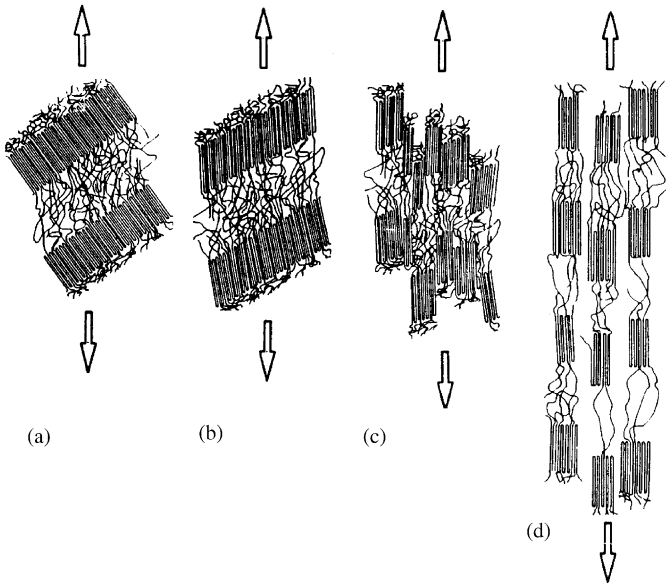

Fig. 1. Morphology change during lamellae stack deformation in a tensile test, after Schultz (1974): (a) interlamellar shear; (b) interlamellar shear plus fine slip in the crystals; (c) coarse slip plus initiation of lamellae breakage; (d) fibrillar state with residual crystalline block portions. Arrows show the loading direction. The imposed deformation increases from left to right.