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Multiscale Modelling of the Mechanical Behaviour of Oriented Semicrystalline Polymers

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Summary: A multiscale numerical model is used to investigate the structure–property relationship for oriented semicrystalline polymers. The basic element in this model is a layered two-phase composite inclusion, comprising both a crystalline and an amorphous domain. An aggregate of preferentially oriented composite inclusions is used in a macroscopic finite element model.

Introduction

The elasto-viscoplastic behaviour of semicrystalline polymeric materials is strongly dependent on the underlying microstructure [1,2]. Semicrystalline polymers consist of both amorphous and crystalline domains. The elastic and the viscoplastic behaviour depend on the percentage crystallinity, the initial crystallographic and morphological texture, as well as the evolution of this microstructure with deformation. For melt-extruded material, a stacked lamellar morphology is often observed. For this material, the mechanical response will depend on the direction of loading with respect to the flow direction, as illustrated by the images in Figure 1.

In recent years, many experimental and modelling studies have focused on understanding the viscoplastic behaviour and the evolution of texture of semicrystalline polymers, e.g. [3-7]. A micromechanically-based model for the constitutive behaviour of semicrystalline polymeric material has been presented in Van Dommelen et al. [8]. The model accounts for both crystallographic and morphological texture, the latter corresponding to the orientation distribution of the lamellar interface normals. A three-level modelling approach was used to study intraspherulitic deformation and stresses for semicrystalline polyethylene [9]. The current work builds on these recently developed models by using this micromechanical framework for the simulation of the mechanical behaviour of oriented high density polyethylene (HDPE), depending on the initial microstructure. A three-level modelling approach is used to study the behaviour of oriented tensile bars.

Model description

The constitutive behaviour of semicrystalline material is modelled by an aggregate of two-phase composite inclusions. This composite inclusion model, which is discussed in detail in [8], is concisely summarized in this section. Each inclusion consists of a crystalline and an amorphous phase. A microstructural elasto-viscoplastic constitutive model is defined for both the crystalline and the amorphous phase.

The crystalline domain of polymeric material consists of regularly ordered molecular chains. The crystal structure shows (i) anisotropic elastic behaviour where the elastic properties, as characterized by a fourth-order anisotropically elastic modulus tensor, are given with respect to the crystallographic directions, and (ii) plastic deformation governed primarily by crystallographic slip on a limited number of slip planes [2,11], which is described by a rate-dependent crystal plasticity model.

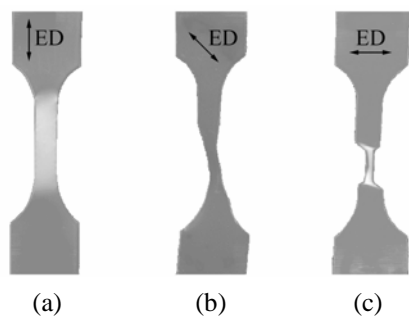


Figure 1: Influence of extrusion direction (ED) for high density polyethylene in tensile tests.

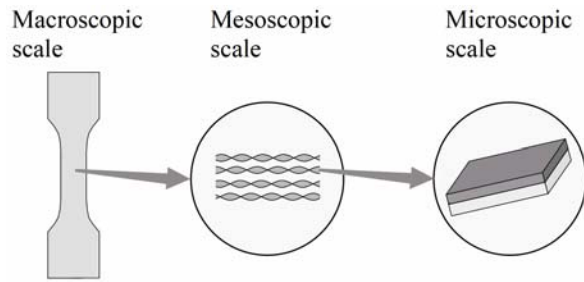


Figure 2: Schematic illustration of the multiscale model.

The amorphous phase of semicrystalline polymeric material consists of an assembly of disordered macromolecules, which are morphologically constrained by the neighbouring crystalline lamellae. The elastic deformation of the amorphous domains is modelled by a generalized neo-Hookean relationship. A relatively strain rate-insensitive power law relation between an effective shear strain rate and an effective shear stress is used [6]. The plastic rate of stretching is defined by an associated flow rule. The Arruda–Boyce eight-chain network model of rubber elasticity [12] is used to account for orientation-induced strain hardening [13,14].

The mechanical behaviour at the mesoscopic level is modelled by an aggregate of layered two-phase composite inclusions as was proposed by Lee et al. [6,7] for rigid/viscoplastic material behaviour. Each separate composite inclusion consists of a crystalline lamella which is mechanically coupled to its corresponding amorphous layer. The stress and deformation fields within each phase are assumed to be piecewise homogeneous, however, they will differ between the two coupled phases. The inclusion-averaged deformation gradient and the inclusion-averaged Cauchy stress are defined as the volume-weighted average of the respective phases. It is assumed that the crystalline and amorphous components remain fully mechanically coupled. Interface compatibility within the composite inclusion and traction continuity across the interface are enforced. To relate the volume-averaged mechanical behaviour of each composite inclusion to the imposed boundary conditions for an aggregate of inclusions, a hybrid local–global interaction law is used [8].

A distinction between three different scales is made, as is schematically depicted in Figure 2. Whereas the composite inclusion model is used to relate the microscopic and the mesoscopic scales, a relation with the macroscopic scale is obtained by using the composite inclusion model in each integration point of a finite element (FE) model of the macrostructure, consisting of an extruded tensile bar where the local material behaviour depends on the extrusion direction and conditions. Local anisotropy results from preferential orientation distributions of composite inclusions.

Results

The stacked lamellar morphology commonly observed in extruded semicrystalline materials gives rise to a strong influence of the direction of flow with respect to the loading direction on the stability and localization phenomena in tensile experiments. The multiscale numerical model is used to simulate the effect of a stacked lamellar microstructure on the macroscopic behaviour [10]. Orientational model input (Figure 3(a)-(d)) is based on WAXS experiments on extruded material. The averaged fields of an aggregate, having these preferential orientations, constitute the mechanical behaviour of extruded material. The mechanical response of the aggregate in different deformation modes is shown in Figure 3(e) and (f). Details on the loading conditions are given in [10].

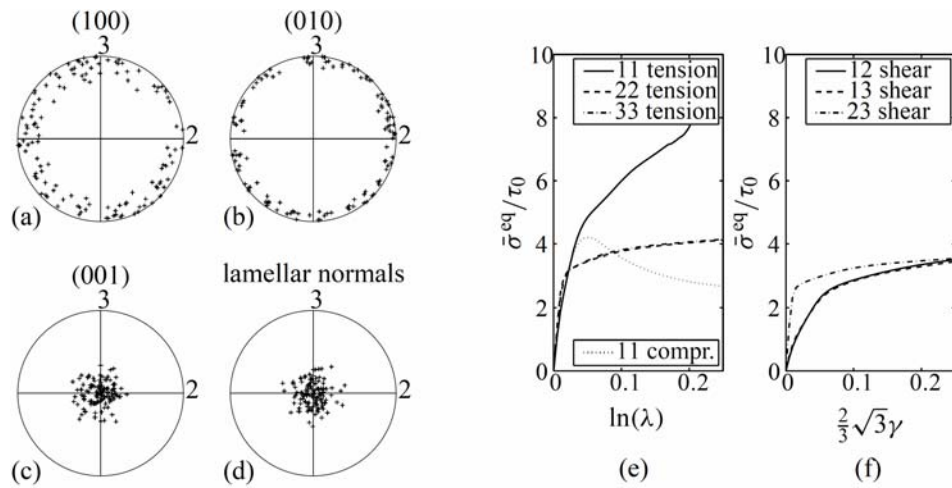


Figure 3: Equal area projection pole figures with (a)–(c) the principal crystallographic lattice directions, and (d) the lamellar normals, and (e), (f) the normalized equivalent mesoscopic stress vs. the imposed deformation for tension and shear, respectively, in the material principal directions. Reproduced from [10].

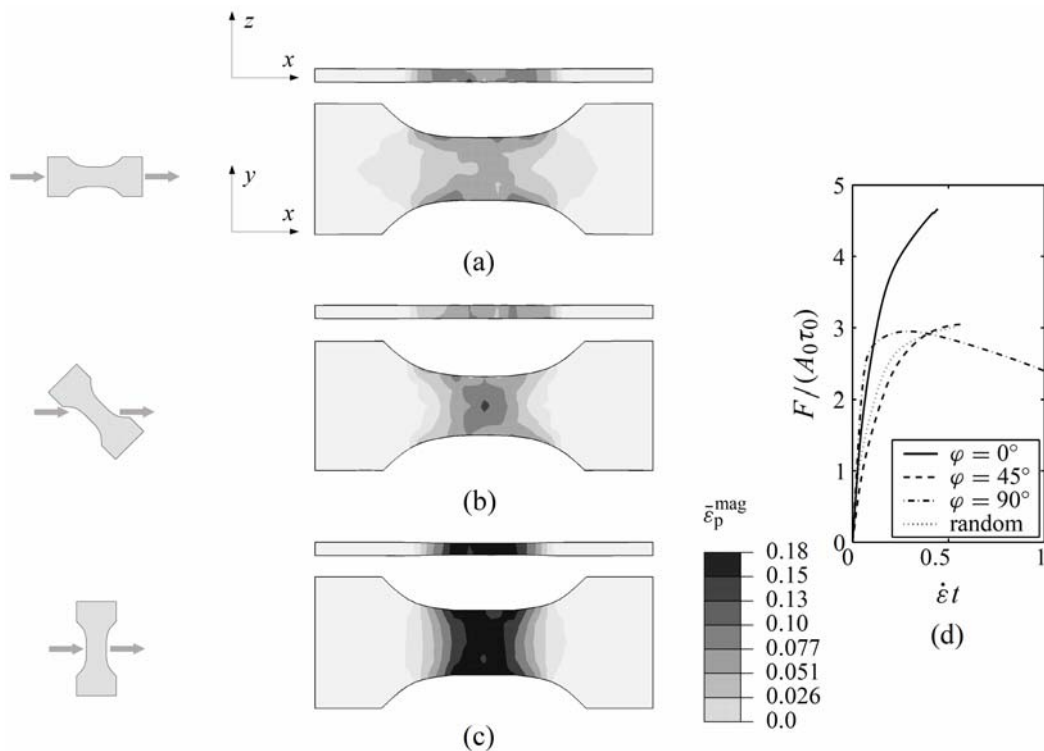


Figure 4: (a)–(c) Magnitude of plastic deformation, at $\dot{\epsilon}t = 0.45$, and (d) macroscopic stress–strain response from simulations of tensile bars of extruded material with various initial angles between the extrusion direction (indicated by the grey arrows) and the loading direction. Reproduced from [10].

A macroscopic tensile bar is described by a finite element model. Results for simulations with various angles between the extrusion direction of the material and the loading direction are given in Figure 4(a)-(c). The microstructure-induced deformation hardening in the extrusion direction that was visible in Figure 3(e), is found to stabilize the macrostructure, when loaded in the flow direction, whereas when loaded perpendicular to the extrusion direction, a neck is formed. This corresponds to the experimentally observed orientation-dependence of extruded semicrystalline material [10].

Conclusions

The deformation of semicrystalline polymeric materials is the result of the interplay of various effects and mechanisms at different levels. A universal prediction of the constitutive behaviour of these materials would require a coupled and detailed modelling of the various deformation mechanisms and criteria for the different failure modes, which is at present still not feasible. In this work, the sole influence of the microstructure, represented by the orientations of the crystalline lamellae, on the mechanical response was investigated using a multiscale model. In each integration point of a finite element model, an aggregate of composite inclusions was used as a representative microstructural element that provides the constitutive behaviour of the material at the mesoscopic level. Material properties were assigned at the microstructural level to both the amorphous and the crystalline phase. Besides these properties, the mesoscopic constitutive behaviour was formed by the crystallographic and lamellar orientations of the composite inclusions. The multiscale model was employed to study the behaviour of material with a lamellar row structure. For extruded material, the microstructure-induced deformation hardening in the extrusion direction was found to stabilize the macrostructure when loaded in the flow direction.

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