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Micromechanics of semicrystalline polymers: Towards quantitative predictions

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ABSTRACT

An initially qualitative two-phase elasto-viscoplastic micromechanical model for the mechanical performance of semicrystalline materials has previously been developed. In the last decade, a series of extensions to this model have been aimed towards quantitative predictions of the response of semi-crystalline polymers based on their microstructure. These developments included extensive experimental characterization and modelling of the yield kinetics, time-to-failure, creep and thermal shrinkage and expansion. This paper gives an overview of the route from the initially qualitative model to a model that quantitatively captures these complex aspects of the mechanical response of a semicrystalline polymer.

1. Introduction

The mechanical response of a polymer material, including the mode of failure and the time-scale on which it occurs, is strongly influenced by the processing conditions. This is particularly true for semicrystalline polymers [e.g. 1,2] in which structural features, such as the degree of crystallinity, crystal type, size and orientation, that strongly influence their mechanical properties, may vary drastically depending on subtle details of the manner in which the polymer is shaped into the final product. For example, shear flow significantly accelerates crystallization kinetics by increasing the amount of nuclei and generates an anisotropic morphology by inducing orientation. Therefore, during processing of a material often an oriented microstructure is formed, leading to anisotropic properties. This anisotropy is intentionally created in fibre spinning, and film casting or film blowing, however, for injection-moulded products, anisotropy is usually an artefact of the processing conditions required to obtain an optimally shaped product. To improve product performance for any of these processes, a fundamental and quantitative understanding of how anisotropic properties, including yield and failure kinetics, depend on the (oriented) structure is required.

Several experimental and modelling studies have focused on understanding the viscoplastic behaviour of semicrystalline polymers [e.g. 3–8]. Macroscopic and phenomenological constitutive models for solid polymers have been successfully developed for rapid and efficient numerical evaluation of the performance of polymer products [e.g. 9–11]. These constitutive models capture the time, stress and temperature-dependent response of polymers, including the effect of their thermo-mechanical history. A micromechanical model that describes the macroscopic response as a function of the morphological structure and constitutive properties of the constituents has the potential to form a predictive tool for the macroscopically anisotropic properties of a semicrystalline polymer with an arbitrary processing-induced microstructure.

Finite-element modelling may be used to describe the mechanical behaviour of a semicrystalline polymer with a known microstructure, i.e. isotropic (spherulitic) or oriented [e.g. 12–14]. These approaches are generally computationally demanding and required cumbersome meshing of the microstructure. Alternatively, various mean-field models have been developed for semicrystalline polymers, such as [3,5,8,15–23]. These micromechanical models often aim at predicting the effective elastic properties based on the polymer's microstructure and in some cases focus on the more complicated yield behaviour as well. An elasto-viscoplastic micromechanical model for semicrystalline polymers was developed by the authors [24–26]. The basic

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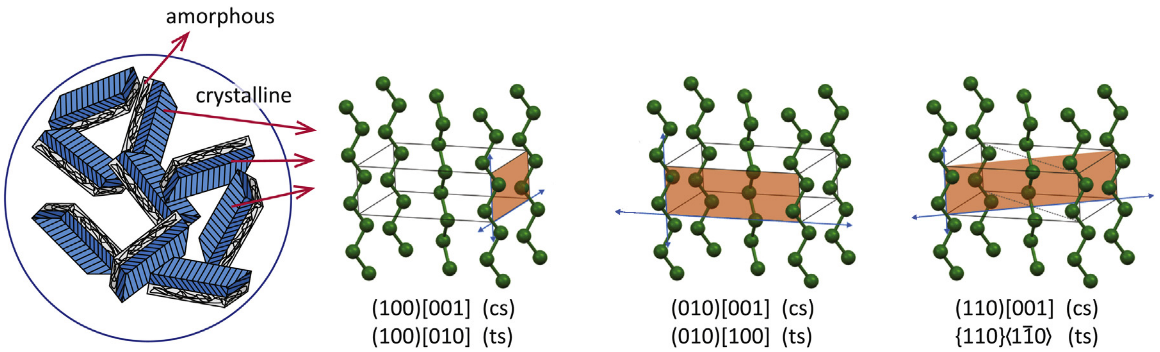


Fig. 1. An aggregate of *composite inclusions* (left) and the six physically different types of slip systems in a polyethylene crystal (right), with "cs" denoting chain slip and "ts" indicating transverse slip.

element in this model is a layered two-phase structure, comprising both a crystalline and an amorphous domain as developed by Lee et al. [5,15] for rigid viscoplastic semicrystalline materials. Initially, the application of these micromechanical models has been mostly limited to systems with a spherulitic and thereby macroscopically isotropic structure (whereas most polymer products have an intrinsically oriented structure) and was aimed at obtaining a qualitative description of the mechanical response [e.g. 14,24,27]. Further research has focused on improving the quantitative abilities of the multiscale micromechanical model, in particular for the stress-dependence of the rate of plastic deformation, i.e. the yield kinetics [28–30]. Recent efforts were successful in providing a quantitative description of macroscopic yield and failure kinetics, also for oriented material [31,32]. In this paper, an overview is given of the development of the so-called *composite inclusion* model for semicrystalline polymers from first being a qualitative model, towards a model that quantitatively predicts the response of these materials.

2. A qualitative model for semicrystalline polymers

2.1. Composite inclusion model

A rigid-plastic mean-field micromechanical model for semicrystalline polymers, referred to as the *composite inclusion* model, was proposed in 1993 in the pioneering work of Lee et al. [5,15] and was used to predict the texture evolution in these materials. The basic element in this model was a two-phase layered structure consisting of a crystalline and an amorphous phase. This concept was later extended to elasto-viscoplastic behaviour by Van Dommelen et al. [24]. In this concept, the response of the semicrystalline material is modelled as an average of an aggregate of these two-phase composite inclusions (see Fig. 1). Within each composite inclusion, the two phases are assumed to be kinematically compatible and in equilibrium across the interface and a hybrid local–global interaction law is used to relate the volume-averaged mechanical behaviour of each composite inclusion to the imposed boundary conditions for an aggregate of inclusions.

Since the crystalline domain consists of regularly ordered molecular chains, in [24] the response of these domains was modelled as anisotropic elastic in combination with plastic deformation governed by crystallographic slip on a limited number of slip systems and for which a rate-dependent crystal plasticity model was used. It should be noted that in contrast to metallic materials, for polymer crystals, the various slip systems are usually physically distinct (for example, the slips systems of a polyethylene crystal are shown in Fig. 1) and therefore have different properties. The amorphous phase of semicrystalline polymeric material consists of an assembly of disordered macromolecules, which are morphologically constrained by the neighbouring crystalline lamellae. In [24], the elastic deformation of the amorphous domains was modelled by a generalized neo-Hookean relationship in combination with a viscoplastic relation and an eight-chain network model to account for orientation-induced strain hardening. For both the slip systems and the amorphous domains, the viscoelastic behaviour was modelled with a power law relation.

2.2. Application to HDPE

This elasto-viscoplastic model was used to describe the macroscopic response of spherulitic (and therefore initially isotropic) high density polyethylene (HDPE), including the effect of crystallinity and to study micromechanical deformation mechanisms. In particular, the intra-spherulitic deformation mechanisms were studied in a multi-scale effort in [27] and the effect of an oriented microstructure in extruded HDPE was qualitatively modelled in [25].

3. Towards quantitative predictions

3.1. Yield kinetics of isotropic HDPE

The next phase in the development of the composite inclusion model was directed towards the quantitative prediction of the yield and post-yield behaviour in semicrystalline polymers during large deformations at different strain rates. A critical factor for this is the stress-dependence of the rate of plastic deformation, the yield kinetics. The kinetics of the macroscopic plastic flow strongly depend on the slip kinetics of the individual crystallographic slip systems. Therefore, an accurate quantitative prediction requires a proper description of the rate-dependence of slip along crystallographic planes. As a first step in achieving this goal, the previously used viscoplastic power law relation was replaced with an Eyring flow rule, which more closely matches the macroscopically observed response. The re-evaluation of the slip kinetics was performed using a combined numerical/experimental approach and the refined slip kinetics were then validated for uniaxial compression data of isotropic HDPE, for different strain rates [29]. A double yield phenomenon was found in the model predictions and was related to morphological changes that induce a change of deformation mechanism, see Fig. 2. In the case of polyethylene, such a double yield point has also been observed experimentally during both tensile and compressive deformation modes. In literature, several possible mechanisms have been proposed to explain this behaviour, among which different deformation processes for the first and second yield point, often associated with fine slip and coarse slip [33–36]. Even though the composite inclusion model considers only fine slip, it mimics this complex behaviour, where

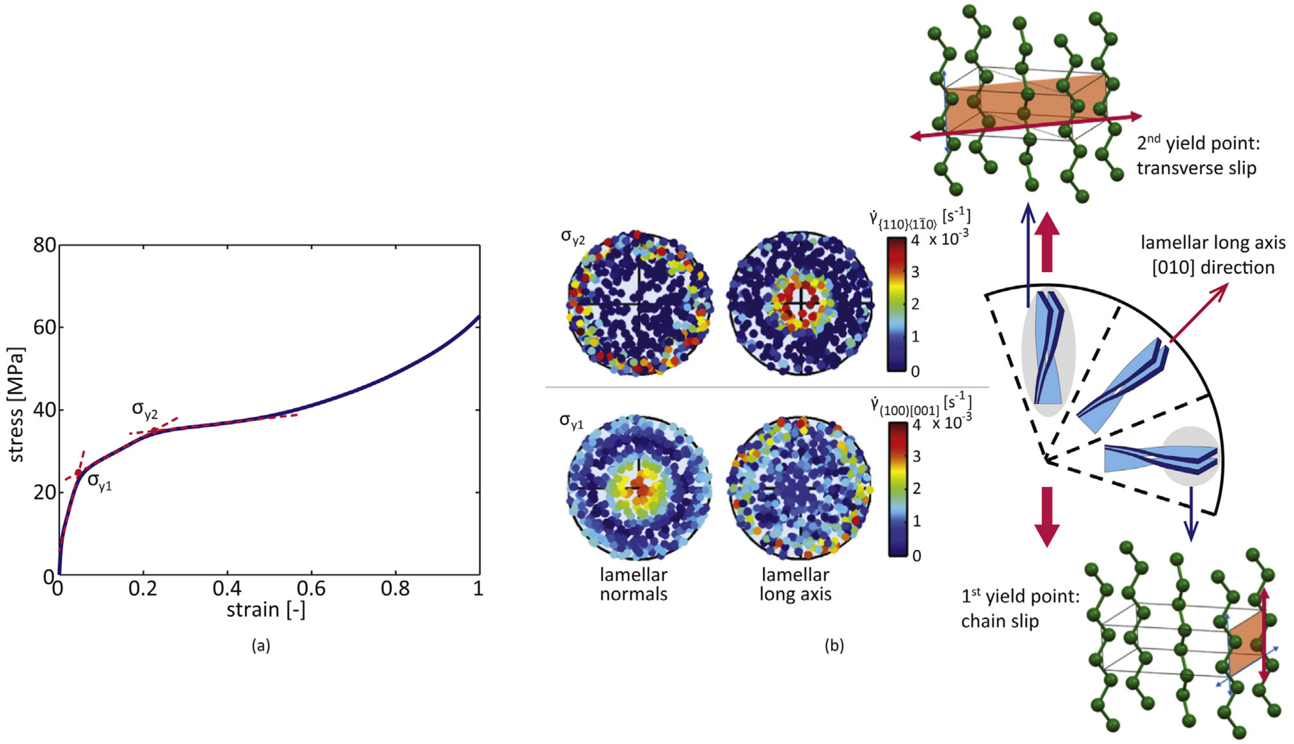


Fig. 2. (a) Double yield behaviour predicted by the micromechanical model for HDPE under uniaxial tension (reproduced from [29]) and (b) microstructural origin of the double yield prediction. The equal area pole figures show the orientation of the two indicated directions of the crystalline lamellae of individual composite inclusions in the aggregate with respect to the loading axis, which corresponds to the viewing direction, and in colour the corresponding shear rate of the indicated slip system for the crystalline phase in that particular inclusion. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of the article.)

it was observed that after the first yield point, a change in the mechanisms occurs and transverse slip systems become active, whereas the primary chain slip mechanism was the dominant process around the first yield point.

The description of the slip kinetics was further refined in order to predict the temperature dependence of the kinetics of yield for polyethylene. The experimental data in Fig. 3 show the presence of two different processes, where one is usually attributed to the crystalline phase and the other to the alpha-relaxation mechanism in the amorphous phase. Also shown in this figure is a prediction of the temperature dependence of the macroscopic yield kinetics as well as time-to-failure in creep experiments with the micromechanical model [30].

In order to predict the response in both tension and compression, a non-Schmid effect (i.e. a dependence on the normal stress σ_n^α acting on the slip system) was included in the slip kinetics [30], which for a single process is then described by:

$$\dot{\gamma}^\alpha = \dot{\gamma}_0^\alpha \exp\left(\frac{-\Delta U^\alpha}{RT}\right) \sinh\left(\frac{\tau^\alpha}{\tau_0^c}\right) \exp\left(\frac{\mu^\alpha \sigma_n^\alpha}{\tau_0^c}\right), \tag{1}$$

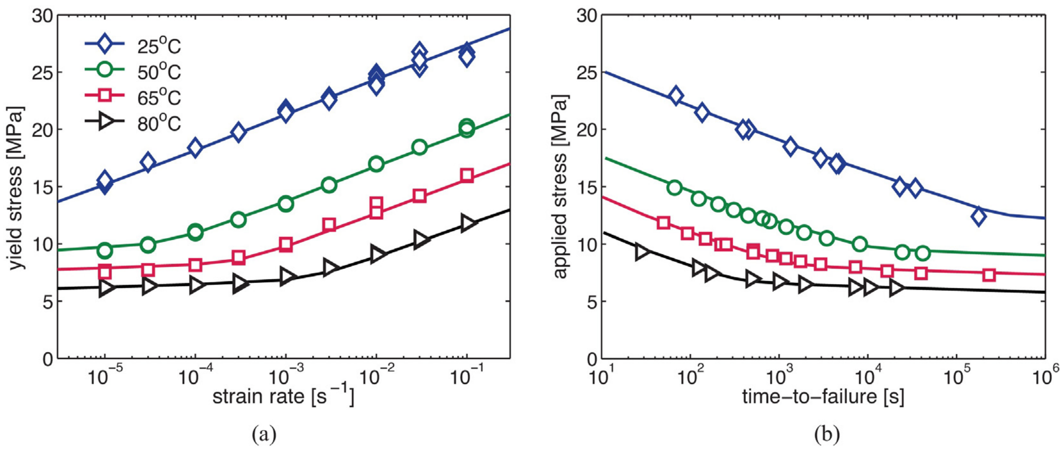
where τ^α is the resolved shear stress on a slip system. The yield kinetics of the amorphous phase was described with a similar relation, where instead of the non-Schmid effect, a pressure dependence was used. However, based on the response of isotropic material, it was not possible to uniquely determine the kinetics of the various slip processes.

3.2. Yield kinetics of oriented HDPE

The mechanical response of extruded and drawn semicrystalline materials, in which a stacked lamellar morphology is commonly observed, depends on the direction of loading with respect to the direction of flow. Plastic deformation and failure are, therefore, both anisotropic. The predictive ability of the micromechanical model, including the characterization of the kinetics of crystallographic slip and amorphous yield based on isotropic material, was next evaluated for oriented high-density polyethylene [37], where the initial morphology of the material was generated based on pole figures from wide-angle X-ray diffraction experiments. Uniaxial loading of an aggregate of composite inclusions with this orientation distribution and with slip kinetics as characterized for oriented material revealed slip activity on particularly the chain slip systems when the loading direction was aligned with the original drawing direction of the material. In contrast, loading perpendicular to the original drawing direction led to slip activity at macroscopic yield on transverse slip systems. This showed the potential of oriented systems for unambiguously determining the yield kinetics of individual slip systems. In doing so, however, it was observed that the presence of an oriented amorphous phase should be dealt with as well.

3.3. Creep response of isotropic and oriented PET

Thereafter, the composite inclusion model was used to understand and predict the effects of the microstructure, as well as loading conditions as time, stress and temperature on the dimensional stability of thin polyethylene terephthalate (PET) foils used as a substrate in flexible electronics. Focussing first on the creep response of isotropic PET, the description of the amorphous domains in the composite inclusion model was further extended. In [38], the amorphous domains are described with a constitutive model for glassy polymers that is referred to as the Eindhoven Glassy Polymer (EGP) model [11,39] and which consists of a combination of viscoelastic Maxwell elements with neo-Hookean-like elasticity and a non-linear viscosity, which is temperature and stress dependent. The stress dependency is described using the



(a) (b)

Fig. 3. Temperature dependence of (a) yield kinetics and (b) time-to-failure of HDPE under uniaxial tension obtained experimentally (markers) and predicted by the micromechanical model (solid lines).

Reproduced from [30].

Eyring flow model and temperature dependency using the Arrhenius law.

A pre-stretching of the amorphous phase was incorporated in the model to describe the anisotropic tensile and creep response of oriented PET foils based on their microstructure [31]. The experimentally measured and predicted anisotropic creep response is shown in Fig. 4, with a higher creep compliance in transverse direction (TD) than in machine direction (MD). The presence of a pre-orientation in the amorphous domains was found to be crucial for a correct description of the creep response for different loading directions.

3.4. Thermo-mechanical response of PET

The pre-deformation of the amorphous domains also drives irreversible deformation upon heating under stress-free conditions, sometimes referred to as a shape memory effect. To simulate the behaviour of the film at high temperatures and to model reversible and irreversible thermal deformation including the

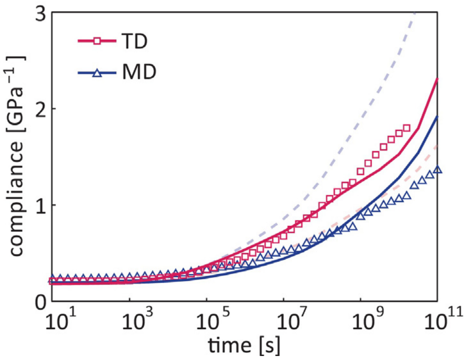


Fig. 4. Experimentally obtained and predicted creep response of oriented PET foil for an applied tensile load of 5 MPa in machine direction (MD) and transverse direction (TD). Reproduced from [31]. The dashed lines show the model result in the absence of a pre-orientation in the amorphous phase.

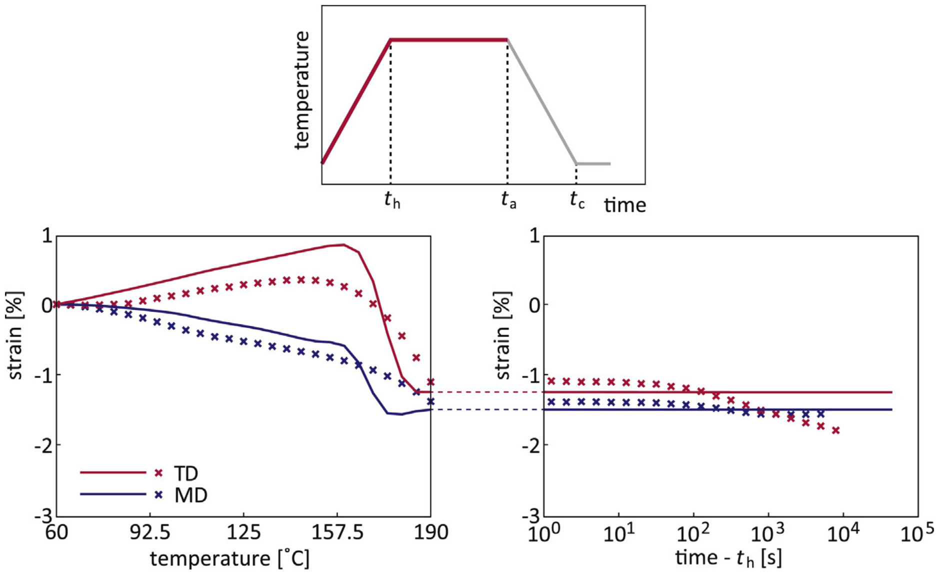


Fig. 5. Expansion and shrinkage in two principal directions of a PET foil upon heating (left) and subsequent annealing (right) as obtained experimentally (markers) and predicted by the micromechanical model (solid lines). The temperature history is schematically shown in the top figure.

Reproduced from [32].

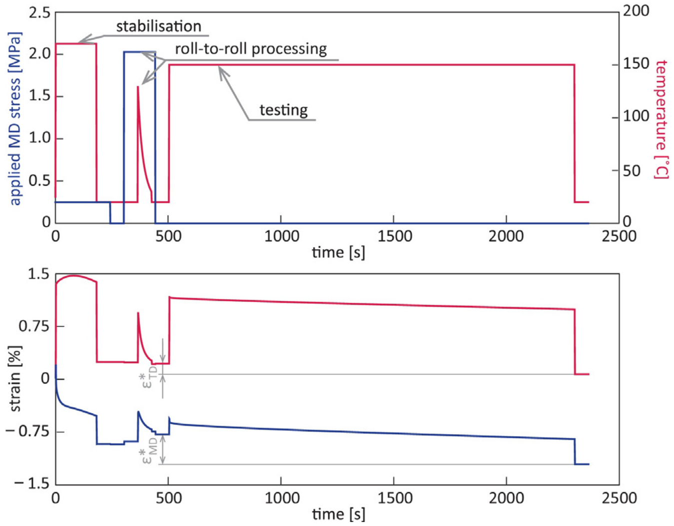


Fig. 6. Complex loading conditions representative for a roll-to-roll lithographic process (top) and the predicted strain evolution in two principal directions (bottom). After [41].

combination of thermal expansion and shrinkage and the effect of the heating rate, thermal expansion was incorporated in the micromechanical model for both phases, as well as a relaxation process for the internal pre-stress in the non-crystalline phase [32,40]. This model was then applied to oriented PET samples that were thermally loaded under nearly stress-free conditions by either increasing the temperature at a low constant heating rate, followed by an annealing stage or by fast heating followed by annealing and fast cooling. The resulting in-plane deformation of the foil in the two principal directions upon controlled heating and annealing is shown in Fig. 5. The model qualitatively describes the experimentally observed response with initially a thermal expansion, followed by shrinkage. Experimentally, two different shrinkage processes were observed in the PET foils, which were described by two pre-deformation modes in the model, where for each mode only one relaxation time was used.

3.5. *Validation for complex loading conditions*

To validate the model under more complex loading conditions, it was used to simulate the film behaviour during various lithographic processing steps, including heat stabilization and roll-to-roll processing [41], the result of which is shown in Fig. 6. Combined thermal shrinkage effects and creep in different directions were predicted rather well, for various processing conditions. However, some deviations still existed and were attributed to an inaccurate description of thermal expansion of the individual phases, which was still assumed to be isotropic for the (oriented) amorphous phase.

4. Conclusions and outlook

In many applications, semicrystalline polymers possess a strongly, processing-induced, oriented amorphous/crystalline microstructure and in turn, the performance of these materials is highly affected by this structure. Micromechanical models that take this morphology into account have the potential to predict the response of a semicrystalline polymer for an arbitrary structure based on a generic characterization of its constituents. The development of such a model is a challenging and complex task because of the presence of many different deformation processes (e.g. crystalline slip or amorphous processes) with each their own properties and with an intricate interaction between them.

In the original work of Lee et al. [5,15], the amorphous/crystalline interaction was captured by a two-phase basic element in which the two phases interact mechanically across an interface. This element was referred to as a *composite inclusion* and has proven to be a powerful concept. It was the basis for many micromechanical models for semicrystalline polymers afterwards. Initially, this approach was used to predict texture evolution and later also yield behaviour and other aspects of the mechanical response, but often in a qualitative manner.

Over the last decade, based on extensive experimental characterization, the contribution of the individual processes was determined and several extensions or refinements to the so-called *composite inclusion* model were made. Initially, the emphasis was on the kinetics of the various crystalline slip systems, but also the importance of the contribution of the amorphous phase became apparent, in particular for oriented material, for which the amorphous network can be in a pre-stretched state. The significance of this oriented amorphous phase is also manifested for low stress/high temperature conditions, where irreversible deformations, sometimes referred to as a shape-memory effect, occur. Recently, for the first time, the performance of this elaborate micromechanically-based model for the mechanical response of a semicrystalline polymer was scrutinized for complex loading conditions involving various thermo-mechanical loading sequences [41]. On many occasions, the model was also used to simultaneously understand and unravel the microscopic deformation mechanisms and the role of the semicrystalline microstructure.

Over the years, the *composite inclusion*-type models have evolved into a powerful approach for prediction of the mechanical response of semicrystalline polymers, but at the same time, the high complexity of them makes their characterization for an arbitrary material challenging. In the model, the kinetics of the individual deformation processes such as crystalline slip are described in a (at that level) phenomenological manner. The physical origin of these slip kinetics requires further interpretation, for which molecular modelling efforts could be of benefit. Although pre-orientation of the amorphous phase has been incorporated, this was done in an oversimplified way, with isotropic elastic behaviour and thermal expansion and anisotropy only through the pre-stretch. For application to non-isothermal conditions, it was found that the current description of thermal expansion, in particular for the amorphous domains, needs further improvement. Also for isothermal loading, a critical evaluation of the model performance has shown the importance of the anisotropy of the amorphous phases. The downside of this is that the state of pre-orientation must be characterized for each set of processing conditions separately. A relation between these conditions and the pre-stretch of the amorphous network would greatly enhance the applicability of the model.

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