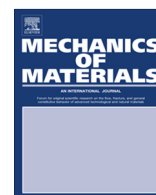




ELSEVIER

Contents lists available at [ScienceDirect](http://www.sciencedirect.com)

## Mechanics of Materials

journal homepage: [www.elsevier.com/locate/mechmat](http://www.elsevier.com/locate/mechmat)

# Modeling of spherulite microstructures in semicrystalline polymers

H. Emre Oktay<sup>a</sup>, Ercan Gürses<sup>b,\*</sup><sup>a</sup> Department of Civil Engineering, Middle East Technical University, Ankara, Turkey<sup>b</sup> Department of Aerospace Engineering, Middle East Technical University, Ankara, Turkey

## ARTICLE INFO

## Article history:

Received 28 June 2014

Received in revised form 6 April 2015

Available online 29 April 2015

## Keywords:

Semicrystalline polymers

Spherulite

Viscoplasticity

Elasticity

FEM

## ABSTRACT

Semicrystalline polymers are composed of crystalline structures together with amorphous polymer chain networks and therefore they exhibit deformation mechanisms of both crystalline materials and amorphous polymers. One of the most common microstructures observed in semicrystalline polymers is the spherulite microstructure in which crystalline lamellae are embedded in a matrix of amorphous material and grow out from a common central nucleus in radial directions. The mechanical behavior of semicrystalline polymers is strongly dependent on the underlying spherulite microstructure. Therefore, characterization of the deformation of spherulites is very important to understand the mechanical behavior of semicrystalline polymers. In this work, we propose a new FEM-based model for semicrystalline polymers which explicitly discretizes the spherulite microstructure consisting of crystalline and amorphous phases. In the model, a viscoplastic crystal plasticity model is employed for the crystalline phase, whereas 8-chain model is employed for the amorphous phase. The model captures the evolution of inhomogeneous plastic deformation activity in a spherulite microstructure, as well as the important features of the spherulite deformation reported in the literature.

© 2015 Elsevier Ltd. All rights reserved.

## 1. Introduction

Polymers, being the typical constituent of plastics in industry, have wide range of application areas in modern life. Among polymers, semicrystalline polymers (SCP) is a subset that gains significant interest owing to their remarkable deformability and toughness, good impact strength, very low gas-permeability and superior wear resistance. Notable examples of semicrystalline polymers being high-density polyethylene (HDPE), ultra high molecular weight polyethylene (UHMWPE), Nylon-6, poly(ethylene terephthalate) (PET), isotactic polypropylene (iPP), semicrystalline polymers have been used in applications

such as electrical insulation systems and substrates for flexible electronic devices to plastic bags, piping systems, liquid and gas containers.

Semicrystalline polymers are composed of crystalline structures alongside amorphous polymer chain networks and they exhibit deformation mechanisms of both crystalline materials and amorphous polymers. They can be considered as two-phase materials consisting of a soft amorphous phase and a hard crystalline phase, where the percentage of crystalline phase can normally vary from 10% to 80%. Complicated and hierarchical microstructure of semicrystalline polymers results in deformation mechanisms that involve complex and multistage processes. There is general consensus in literature (Lin and Argon, 1994; Oleinik, 2003) that, despite the strong covalent bonding of the polymer chains, crystallographic slip that is akin to that observed in metals is the predominant

\* Corresponding author.

E-mail addresses: [emre.oktay@metu.edu.tr](mailto:emre.oktay@metu.edu.tr) (H.E. Oktay), [gurses@metu.edu.tr](mailto:gurses@metu.edu.tr) (E. Gürses).

plastic deformation mechanism in the crystalline phase. Nevertheless, the existence of the polymer chains decreases the number of independent slip systems and therefore constrains the accommodation of arbitrary plastic deformations. Therefore, the complicated interaction of amorphous and crystalline phases is important to understand the overall behavior of the material.

One of the most common microstructures observed in melt crystallized semicrystalline polymers is the spherulite microstructure (Oleinik, 2003). In a spherulite microstructure, crystalline lamellae are embedded in a matrix of amorphous material and grow out from a common central nucleus in radial directions. Ribbon shaped crystalline lamellae are 3–20 nm thick and form spherulites with diameters normally in the range of 2–100 microns.

In development of micromechanically motivated material models, Taylor type homogenization models have proved to be successful especially for highly symmetric metallic crystals. However, Taylor type homogenization is known to be too stiff for crystals that are lacking five independent slip systems, due to insufficient kinematic freedom to accommodate arbitrary plastic deformations. Therefore, Parks and Ahzi (1990) developed a hybrid model where lack of kinematic freedom in plastic straining is modeled in terms of kinematic constraints. They have studied the texture evolution of HDPE and obtained reasonable agreement with experiments even though the amorphous phase of the polymer is fully ignored in their model. Lee et al. (1995) reformulated (Parks and Ahzi, 1990) to obtain a more suitable model for crystals having non-orthogonal lattices such as Nylon-6, PP and PET. Additionally, Lee et al. (1993a) developed a micromechanically based composite model consisting of aggregation of the amorphous and crystalline phases in the form of an infinitely extended sandwich on the grounds that this aggregation is the basic constituent of a spherulite. They proposed three models with different interaction laws, one of which employs a Sachs-like averaging scheme and remaining two employing hybrid averaging schemes, where in all models both crystalline and amorphous phases are modeled as rigid viscoplastic. While chain inextensibility is enforced with constrained crystal plasticity as in Parks and Ahzi (1990), chain alignment and the corresponding anisotropy in the amorphous phase is taken into account through a back-stress tensor computed as in eight chain network model (Arruda and Boyce, 1993) of rubber elasticity. Lee et al. (1993b) employed (Lee et al., 1993a) to study large plastic deformation of HDPE under different straining modes. They have obtained good agreement with experimental observations including macroscopic stress strain behavior.

Later, Van Dommelen et al. (2003b) extended the models of Lee et al. (1993a) by introducing elasticity to constitutive models of both crystalline and amorphous phases under a Taylor-Sachs hybrid interaction law. They have studied the influence of the degree of crystallinity on the macroscopic stress strain behavior and obtained reasonably good predictions for initial modulus and yield strength. Sedighiamiri et al. (2011) aimed to add quantitative prediction capability to Van Dommelen et al. (2003b) for yield and post-yield behavior of semicrystalline

polyethylene. To this end they have re-evaluated slip kinetics of slip systems and replaced originally employed power law with an Eyring flow rule in order to capture rate dependence of slip more properly and obtained promising agreement with experimental stress strain behavior of HDPE. Sedighiamiri et al. (2012) enhanced (Van Dommelen et al., 2003b; Sedighiamiri et al., 2011) to provide quantitative relation between short and long term deformation kinetics of semicrystalline polymers, by adding a temperature shift function to the Eyring flow rule and a non-Schmid effect to constitutive relation of slip systems. They have obtained promising agreement with creep behavior of polyethylene. Gueguen et al. (2010) and Sedighiamiri et al. (2010) proposed three phase models consisting of crystalline, amorphous and rigid-amorphous phase in between crystalline and amorphous phases to study the elastic properties of PET and HDPE, respectively.

Although these models have an advantage due to the ability to calculate response of specifically preoriented materials as exploited in Van Dommelen et al. (2004), response of a spherulite is not considered explicitly in these studies. One approach to model spherulites with these models is to consider the orientations of radially grown lamellae from the spherulite nucleus via use of representative volume elements (RVE) in a finite element method analysis as Van Dommelen et al. (2003a) employed to study intraspherulitic deformation. Tomita and Uchida (2005) used finite element homogenization method to investigate tensile deformation behavior of HDPE at mesoscopic level as well, under plane strain conditions. In the integration points of finite elements a multi-scale material model that considers chain inextensibility comparable to Van Dommelen et al. (2003a) is employed. They have been able to observe that the chain and lamellae interface directions rotate to align the tensile straining direction. Uchida et al. (2010) used representative volume elements to study multi-spherulitic mesostructure with elasto-viscoplastic deformation behavior of semicrystalline polymer under tensile loading. They have found that mesoscopic response is almost independent of the number of spherulites in the RVE. Uchida and Tada (2013) employed a multi-scale composite model in FEM based homogenization framework of spherulites by assigning properly oriented composite constitutive models to the integration points of elements forming a three dimensional spherulite structure. They have studied elasto-viscoplastic deformation behavior of HDPE under different loading conditions and considered influence of degree of crystallinity as well. They have obtained results that represented experimental characteristics. Nevertheless, although these studies take into account the radial orientations of lamellae within a spherulite, they do not account for the interaction of crystalline and amorphous phases deforming within a spherulite consistently as a whole, since interaction between laminar composite constitutive models in separate integration points does not exist.

Yang and Chen (2001) developed a model employing a continuous orientation distribution of chain axes. Only crystalline phase is considered in the model, amorphous phase is taken into account via its influence on crystalline slip. With this 3D model, they have obtained reasonable

Download English Version:

<https://daneshyari.com/en/article/797516>

Download Persian Version:

<https://daneshyari.com/article/797516>

[Daneshyari.com](https://daneshyari.com)