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Numerical Analysis of Mechanical Behavior of Semi-Crystalline Polymers Based on Continuum Damage Mechanics

H. Mehdipour [1], M. Ganjiani[1]*

[1] Mechanical Engineering Department, University of Tehran, Tehran, Iran

ABSTRACT: In the current study, semi-crystalline polymers and their properties are introduced, and then a mechanical model is precisely presented in order to predict the behavior of these materials. In this model, a material point of the semi-crystalline polymer is considered as an aggregate of inclusions of two phases, namely, the crystalline and the amorphous phase, with the interface plane of these two phases. Constitutive equations of each phase are demonstrated. A numerical algorithm is presented for solving the constitutive equations of each phase, in stages. Moreover, the general behavior of the material is determined in terms of each phase behavior using volume averaging. Because of the availability of the material parameters for polyethylene, this material has been taken into account. Obtained numerical results are reported and compared to that of previous models. After supporting the validity of the presented model, the effect of some material parameters including crystalline phase damage rate, release parameter, amorphous phase damage rate, saturation damage, rubber shear modulus, and amorphous phase strength on polyethylene behavior has been discussed in details.

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1- Introduction

Semi-crystalline polymers are a group of polymers that have a regular molecular structure. These polymers are widely used in the industry. Polyethylene and polypropylene, which make up half of the plastic material in the world, are examples of these kinds of materials. Therefore, the analysis of the mechanical behavior of these materials has always been important and considered. Various models have been proposed to predict the mechanical behavior of these materials. A group of these models is the analysis of material behavior by continuum damage mechanics point of view. In this method, the material behavior is predicted by introducing a damage variable based on structural properties of the material and coupling it with the constitutive equations.

In general, models of deformation mechanisms in semi-crystalline polymers submitted based on the microstructure fall into two general categories:

• Models based on phenomenology: Some researchers have presented models that have a purely phenomenological point of view [1-5]. The researchers have correctly predicted nonlinear behavior of semi-crystalline polymers using mathematical functions. These functions include coefficients for the strain rate and temperature.

• Models based on Physics: In these models, semi-crystalline polymers are considered as an aggregate of inclusions of crystalline and amorphous layers which are randomly oriented. These models have the ability to simulate material behavior in a macroscopic point of view [6-11].

The purpose of this paper is to consider semi-crystalline polymers as an aggregate of inclusions (crystalline and amorphous phases) and present a constitutive model based on Lee et al. [12, 13] model. The damage variable in the governing equations coupled not only for the crystalline phase but also for the amorphous phase and hardening is also considered for both phases. Then a numerical algorithm is proposed to solve the equations.

*Corresponding author's email: ganjiani@ut.ac.ir

2- Methodology

As shown in Fig. 1, the semi-crystalline polymer is modelled as a collection of inclusions. Each inclusion consists of crystalline material lying in a thin lamella attached to an amorphous layer. The interface region interconnecting the two phases is the plane through which loads are carried and transferred. It is assumed that the constitutive model contains complete information about the mechanical behavior and degradation processes of each constituent. After modeling two phases independently, the inclusion behavior is found by applying some equilibrium restrictions along the interface plane.

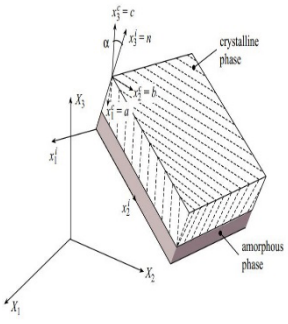

Fig. 1: Semi-crystalline inclusion schematic

In the present model, crystalline phase damage is defined as the separation of crystallographic plates as well as the amorphous phase damage as the growth of cavities.

Also, the numerical solution involves a twice-iterative scheme. The first iteration occurs in the calculation of the stress state of each one of the inclusion constituents; the amorphous and crystalline phases. The second iteration takes place to determine the stress state that satisfies overall equilibrium in the aggregate at time t_{n+1}. This last algorithm uses a constant time increment, Δt, where $\Delta t=t_{n+1}-t_n$. After convergence of the general solution at time increment t_n, damage parameter, the crystal orientation, and texture are updated and the problem solves in the next time increment.

3- Discussion and Results

Using the proposed model and algorithm, the mechanical behavior of polyethylene as a semi-crystalline polymer was obtained under uniaxial tension loading and compared with the results of experiments of Ref. [14] and previous models [10,13]. Also, the effect of the physical parameters of this material on its mechanical behavior is studied.

The results obtained from the present model, as well as the models of Lee et al. [12], Nikolov et al. [10], Alvarado et al. [15] and the results of the G'sell's experiments [14], are presented for equivalent stress in terms of the equivalent strain in Fig. 2.

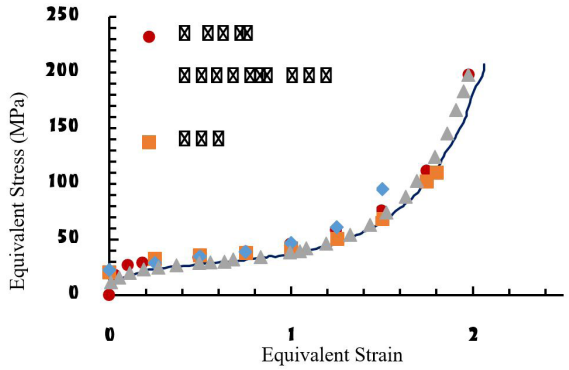

Fig. 2:Polyethylene Stress-Strain diagram for uniaxial tension

As seen in Fig. 2, this model is not only in good agreement with previous results, but, like the Alvarado model, it has the ability to predict stress for larger strains as well.

After validation of the proposed model, the effect of some parameters such as crystalline phase damage rate, release parameter, amorphous phase damage rate, saturation damage, rubber shear modulus and amorphous phase strength on the polyethylene behavior have been investigated.

4- Conclusion

The use of Continuum Damage Mechanics in the constitutive equations of the semi-crystalline polymer makes the proposed model more flexible than previous models and allows us to study the effect of different physical parameters on the material behavior.

In this model, the ability to analyze and predict the behavior of polyethylene was obtained by linking the microstructural properties to the overall behavior of matter. It was also observed that Morphological changes in the structure of matter led to different behaviors in large dimensions.

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