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Modeling of the mechanical behavior of amorphous glassy polymer based on the quasi-point defect theory—Part II: 3D formulation and finite element modeling of polycarbonate

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ABSTRACT

A three-dimensional formulation of the quasi-point defect theory has been developed and the corresponding constitutive equations have been implemented in the finite element package Abaqus, via the writing of an UMAT file. The proposed tool has been completed to support the large strain description and thus can perform a general structure calculation. Referring to a unique set of parameters identified in the part I of this paper for glassy amorphous bisphenol-A polycarbonate (PC-BPA), various commonly used tests were then considered as structural patterns and modeled. The whole mechanical response as well as localization phenomena measured via video technique is well predicted by the calculations. These results also highlight the need to consider the spatial dimension in a sense that the mechanical behavior up to large strain is related to structural modifications, especially for materials such as amorphous polymers that exhibit yield, softening and hardening intrinsic phenomena.

1. Introduction

Until now, the conception procedure of thermoplastic polymer components for industrial applications based on finite elements calculation suffered from the lack of adapted and robust constitutive equations to describe the peculiar mechanical behavior of this kind of material. Indeed, its complex intrinsic behavior is hardly reproduced in a wide set of external conditions. Two different types of models have been developed up to an implementation in a finite element code in order to describe such behavior.

The first type of models is purely phenomenological. Depending on the complexity of the proposed equations and of the number of used parameters, these models can simulate a more or less large number of experimental conditions, and the assumptions embedded are related to the effects focused on. For instance, Lu and Ravi-Chandar [1] consider an elasto-plastic description via a trilinear model to illustrate the localization phenomena. In many efforts, elasto-viscoplastic description of amorphous polymers are developed for FE calculations [2,3]. Finally, authors of Refs. [4–6] implement a viscoelastic–viscoplastic phenomenological description in their FE code. In those theories, we can point out the lack of physical significance and the possible non-uniqueness of the parameters, even for the most complex and therefore the most complete models. Those limitations compromise the validity of the equations as soon as the experimental conditions are enlarged.

The second type of models aims to consider the microstructure of the polymer (even though phenomenological concepts are included to a certain extend). Many theories consider two distinct internal physical contributions to the total resistance to deformation as initially proposed by Haward and Trackay [7]. The first one is a resistance to flow based on a microstructural scenario [8–10] that leads to the prediction of the yield phenomena. In addition to this flow rule, a network resistance is added, leading to the strain hardening and allowing the model to account for the large strain behavior. This was done by making the analogy between the elasticity of a cross-linked network of flexible chains (rubber) and the hardening of an entangled network of chains that are (locally) relaxed by virtue of shear yielding (hardening in an amorphous glass). More or less refinement in the definition of the active chains, i.e. the number of active polymer "crosslinks" in the strained material has then been considered [11–15]. However, it is noteworthy that most of these models do not propose a global vision of the whole viscoelastic–viscoplastic behavior of amorphous polymer, being essentially interested in its viscoplastic aspect. Recently, Anand and Ames [16] proposed a generalization of this approach. In his model, a set of Kelvin–Voigt elements accounts for the inelastic micro-mechanisms and 31 parameters mostly phenomenological need to be determined. This illustrates the complexity for

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