



Modelling of the mechanical behaviour of amorphous glassy polymer based on the Quasi Point Defect theory—Part I: Uniaxial validation on polycarbonate

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ABSTRACT

This paper is devoted to the modelling of the viscoelasto-viscoplastic behaviour of amorphous polymers based on the Quasi Point Defects (QPD) theory. A summarized and unified description of the main assumptions is presented in its scalar formulation to compute the complex viscoelasto-viscoplastic behaviour of an amorphous medium in the glassy state from linear to non-linear ranges. Based on an original scenario for the microstructural reorganization caused by an external thermomechanical stimulus and related to the two main relaxation processes, this theory allows a coherent description of the material response under large conditions of temperature and strain rate by using a single set of material parameters. A convincing validation is performed on a ductile bisphenol-A polycarbonate (PC-BPA) by comparison between computed results and experimental measurements.

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1. Introduction

Compared to ceramics or metals, polymeric materials exhibit specific mechanical behaviour resulting from the fully (amorphous polymers) or partially (semi-crystalline ones) non-crystalline state of the matter. Focusing on amorphous polymers, two types of behaviour can be observed depending on the temperature range. Below the glass transition temperature T_g , the modulus of the material in the glassy state is of a few GPa's. It drastically decreases down to a few MPa's above T_g , where the material stands in its so-called rubber behaviour. This state is highly dependent on the macromolecular nature of the material. Indeed, depending on their length, the polymer macromolecules are more or less entangled, creating temporary crosslinks which delay the flow of the material. For obvious reasons, in most structural applications, amorphous polymers are used in their glassy state. Under such conditions, their non-linear mechanical response is associated with processes characterized by a strong dependence on temperature and strain rate [1–4]. Therefore, modelling approaches must correctly describe their behaviour features in order to allow predictive design of polymer parts.

There are several ways to deal with such a complexity [5]. A convenient one consists in developing phenomenological constitutive equations. Nevertheless, models are usually limited to a given set of experimental conditions with restricted predictive capabilities. The description of the whole mechanical behaviour of

amorphous polymers observed under various loading conditions remains challenging and improvement is often obtained when trying to investigate and account for some structural movements at the origin of the macroscopic strain. More generally, different conceptual scenarios of the macromolecular deformation under stress were proposed depending on the scope of the research. Mainly, two kinds of description are commonly used. In the range of deformation that does not imply residual strain often associated with the yield phenomena, a non-linear “viscoelastic” description is frequently employed [6–12]. These approaches can be indistinctly used for amorphous polymers in the glassy state or for semi-crystalline polymer or filled amorphous polymers in the rubbery state. They are usually phenomenological and derived from Maxwell description. Some of them account for the non-linearity by the use of an internal clock time concept, which leads to an evolution law of the effective time scale. This concept of an internal clock time can be related to physical internal variables, which enable the modelling of the influences of temperature and strain rate [13]. A straight-forward strain rate or temperature dependency of the parameters can also be accomplished to account for the non-linear behaviour [14].

At large deformation, yield, softening and hardening processes also have to be described. Hence, generalized models devoted to this deformation range are essentially “elasto-viscoplastic”, in which one single process describes the yield phenomena associated with the initiation of the “plastic” strain [15–18]. The relevant models found in the literature use a physically based decomposition of the total stress. The yield process is predicted by an intermolecular activation stress based on a single micro-mechanical rearrangement process [19,20], and the deforming entangled

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