Micromechanical modelling of the thermo-mechanical behaviour of semicrystalline polymers

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In flexible electronics, polymeric materials may replace conventional substrate materials as silicon, providing flexibility, and potentially enabling roll-to-roll manufacturing. Polymeric films that are used as a substrate for flexible electronics and which usually have a strongly oriented semicrystalline microstructure, need to satisfy a number of requirements, among which good dimensional stability, also at elevated temperature. This dimensional stability is highly dependent on the internal macromolecular orientation.

This work aims at understanding and predicting the effects of the microstructure, as well as loading conditions as time, stress and temperature on the mechanical response of thin semicrystalline polymer films. For this purpose, a micromechanical thermo-elasto-viscoplastic model is developed to predict the dimensional stability of films when exposed to these loads. The model considers the material to consist of an aggregate of two-phase layered domains, where different constitutive laws are used for the phases [1]. The crystalline phase is modelled with crystal viscoplasticity and the amorphous phase is described as an elasto-viscoplastic glassy polymer, taking account material ageing [2].

The micromechanically-based model is used to describe the mechanical behaviour of amorphous and semicrystalline polyethylene terephthalate (PET) under uniaxial compression and uniaxial tension up to large strains and at different temperatures [3]. The model is used to describe the anisotropic elastic and viscoplastic response of oriented PET films, that is experimentally observed, based on their microstructure [4]. The presence of internal stresses in the material, resulting from material prestretching and heat treatment, is measured and modelled. Using information about the orientation distribution of the crystalline phase, the local thermo-mechanical behaviour is predicted. To demonstrate the applicability of the model to describe the long-term response, the creep behaviour is simulated and compared to experimental data.

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