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Multi-scale modelling of oriented polymer foils

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Objective

The project aim is to understand and predict the effects of time, stress, temperature and humidity on the mechanical response of thin semicrystalline polymer foils during lithographic processing and handling. A multi-scale modelling tool is developed capable to predict dimensional stability of flexible substrates, in particular PEN and PET foils. These foils are used to manufacture plastic electronics, for instance, a plastic memory for RFID or the backplane of a flexible display (figure 1).

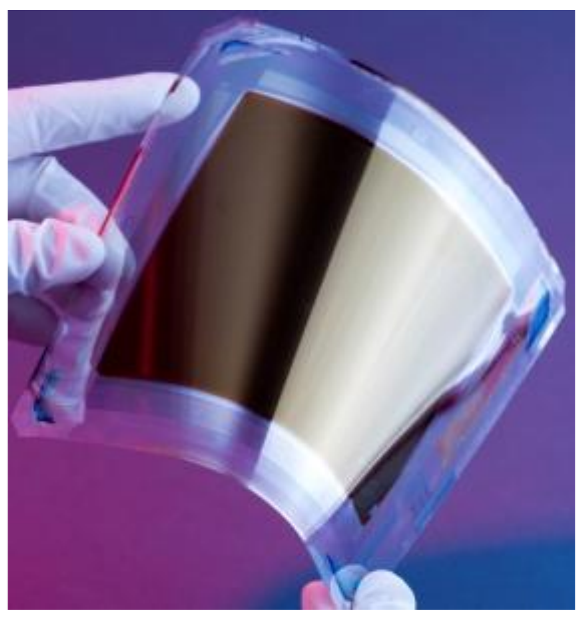

Figure 1. Flexible OLED by PARC.

Modelling approach

The composite inclusion model is a material point model, relating the macroscopic stress and the deformation gradient (figure 2), in which these macroscopic quantities are obtained by volume averaging of local quantities. The microscopic scale is represented by layered domains, which are linked by a hybrid interaction law (between parallel and serial connection of domains). Multi-scale modelling approach is used to obtain a structure-property relationship for oriented material.

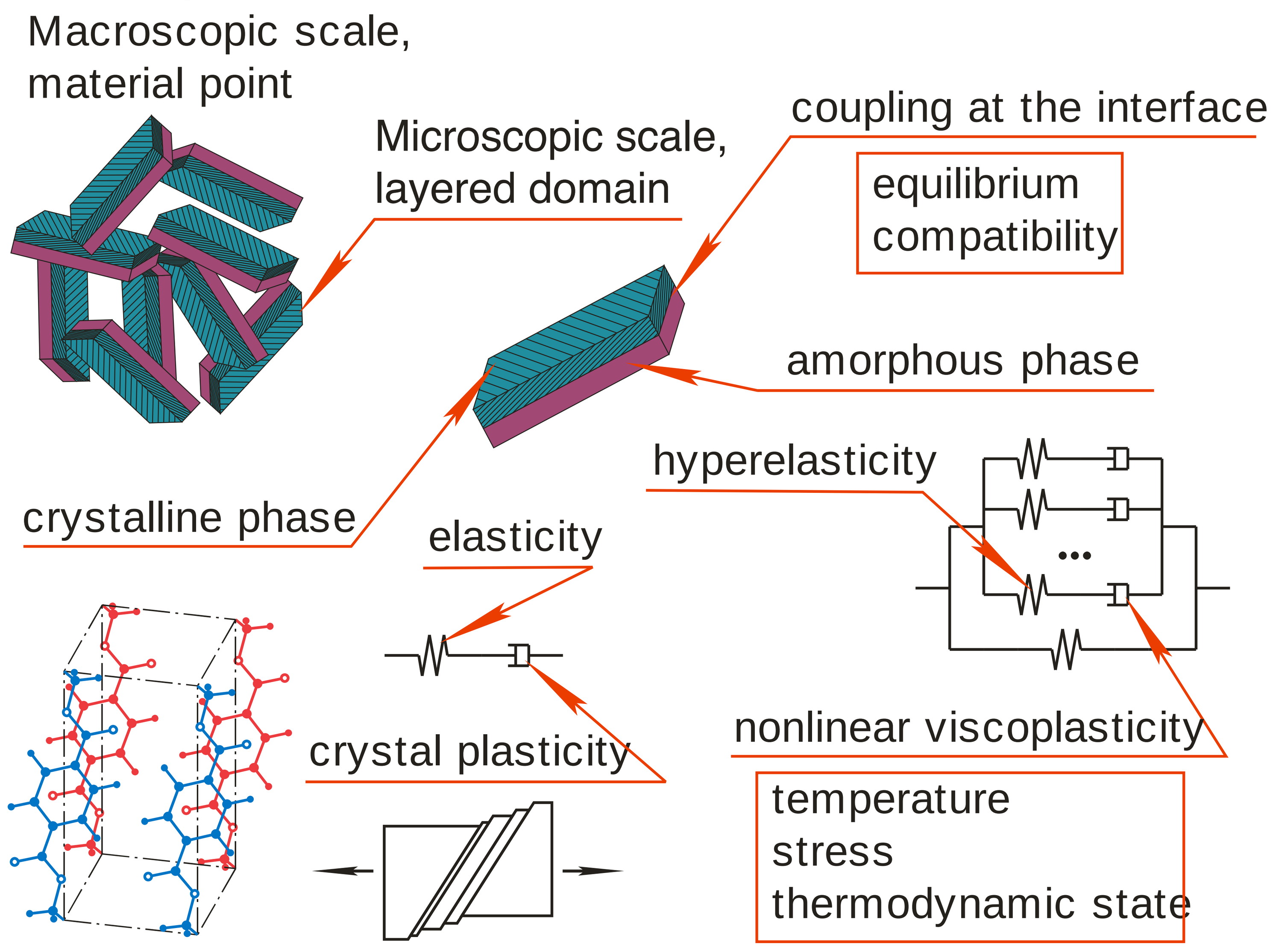

Figure 2. Modelling scheme.

Results

Experimental macroscopic characterisation of short-term and long-term behaviour of the oriented foil was performed establishing degrees of anisotropy and inhomogeneity. Initial parameter identification was performed on isotropic samples, with more precise characterisation obtained using experimental data for orientated foil. Figure 3 demonstrates the ability of the model to simulate the large-strain anisotropic behaviour of PET in the strain rate controlled regime.

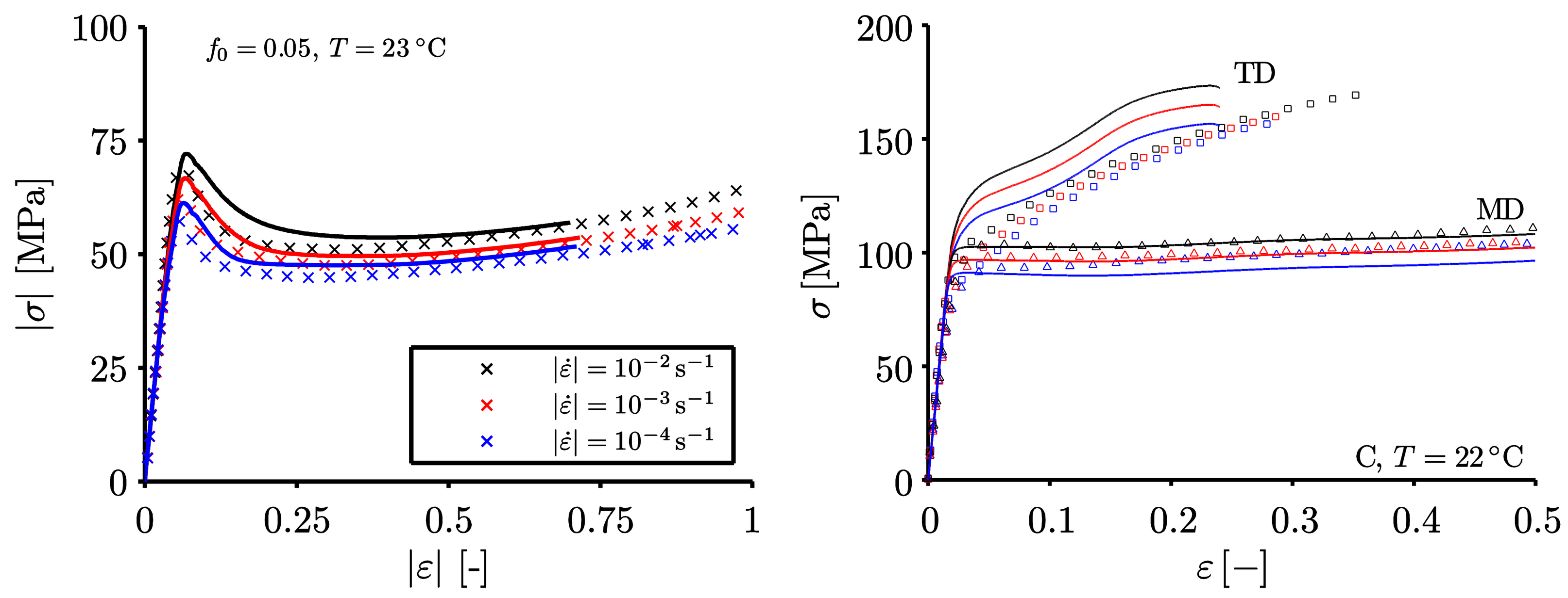

Figure 3. Uniaxial compression of isotropic sample (left) and uniaxial tensile loading of oriented sample (right).

Creep master curves, which were constructed using time-temperature superposition, show a difference in dimensional stability of the foil in the machine direction (MD) and the transverse direction (TD), resulting from the orientation of the crystalline phase created by the production process. If internal anisotropic stresses in the non-crystalline phase (also a result of the manufacturing) are incorporated in the micromechanical model, the long-term behaviour of PET can be predicted, figure 4.

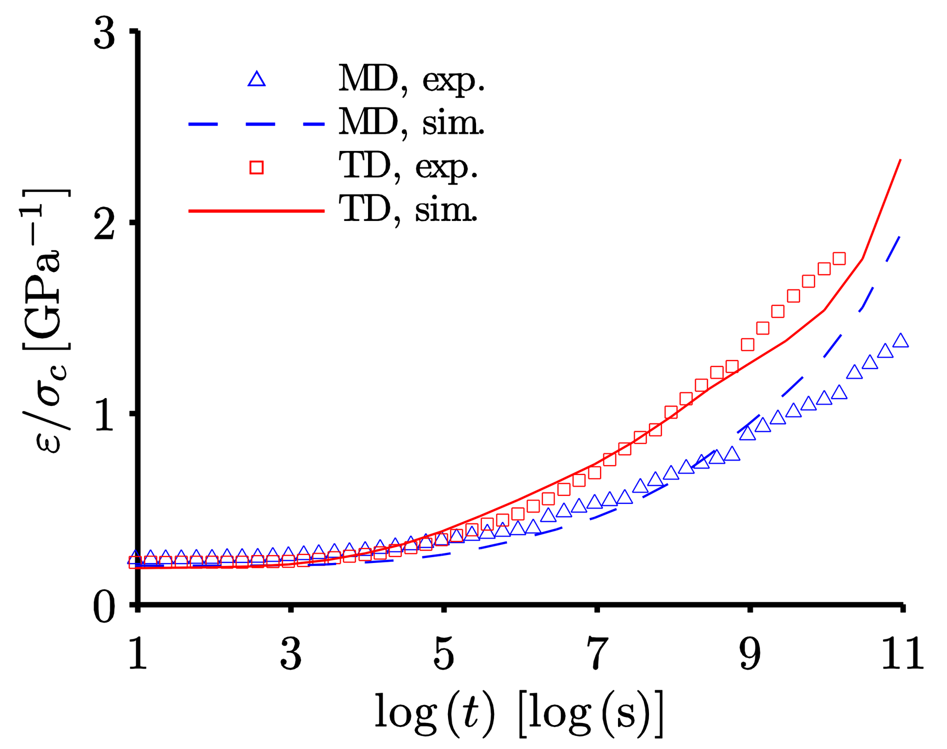

Figure 4. Creep compliance for oriented PET foil at 50°C and applied stress of 5 MPa.

Conclusions

The short-term and long-term macroscopic behaviour at different conditions can be predicted with the composite inclusion model using information about the underlying microstructure. Parameters of the constitutive laws describing the different constituent phases at the microscopic level can be identified from the experimental data.