Continuum mechanical modelling of deformation and failure mechanisms in thermoplastic multilayer composites

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Thomas Seelig

Institute of Mechanics
Kaiserstr. 12
D-76131 Karlsruhe
Tel.: +49 (0) 721/ 608-2071
Fax: +49 (0) 721/608-7990
E-Mail: info@ifm.kit.edu
www.ifm.uni-karlsruhe.de

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Institute of Mechanics, Karlsruhe University, Germany, Seelig@ifm.uni-karlsruhe.de

Summary: The presentation deals with the deformation and failure behaviour of thermoplastic composites which consist of many alternating layers of PC (polycarbonate) and SAN (styrene-acrylonitrile), i.e. a ductile and a brittle glassy polymer. While extensive experimental work has revealed several aspects of the microscopic and macroscopic behaviour [1-2] the present work aims at gaining additional insight from detailed finite element simulations.

Introduction

Thermoplastic composite materials with a regular fine-scale microstructure of many alternating layers of two constituents can be obtained by coextrusion a ductile glassy polymer (e.g. polycarbonate, PC) and a brittle glassy polymer (e.g. styrene-acrylonitrile, SAN). Experiments on PC/SAN multilayer composites have shown that the overall behaviour under tensile loading parallel to the layers varies from early brittle failure to a highly ductile response with increasing PC content [1-2]. The presence of the ductile PC layers of course hinders the unlimited growth of crazes from the brittle SAN. But the key mechanism controlling whether the composite displays an overall brittle or ductile response appears to be the *interaction* between multiple crazing (and subsequent microcracking) in the SAN and shear banding in the PC. Under appropriate conditions, i.e. a sufficient relative thickness of PC layers, a network of crazes (in SAN) and interconnecting shear bands (in PC) is observed that extends throughout a large region of a test specimen and causes a delocalization of damage that results in an overall ductile behaviour.

Aiming at a deeper understanding of the intriguing interplay between microstructure, micromechanisms and overall behaviour, finite element analyses of PC/SAN multilayer composites have recently been performed in [5] and [6] utilising different continuum mechanical descriptions of the crazing process. Here we briefly discuss important issues of the continuum mechanical modelling and focus on the numerical investigation of the effect of relative layer thickness, i.e. volume fraction of PC and SAN, and its implications for the microscopic and overall composite behaviour.

Problem formulation

PC/SAN multilayer composites are modelled here assuming 2D plane strain conditions. A sample (of height h) of the material consisting of several layers as sketched in Fig. 1a is considered and overall loading parallel to the layers is imposed in terms of a macroscopic strain rate $\dot{\bar{\varepsilon}} = \dot{u} / h$ by prescribing the velocity $\dot{u}$ on the upper boundary of the sample. Several equally spaced cohesive surfaces normal to the loading direction are introduced throughout the sample as potential locations of failure (Fig. 1a). While failure in the SAN layers starts by the formation of crazes at a few per cent of strain (treated by the cohesive model discussed in the following section), PC fails only after very large stretching of its molecular network is attained. This causes an incompatibility of the (continuum) deformation in the vicinity of the PC/SAN interface, and Figs.1b-e illustrate how this is handled within the framework of the finite element model.

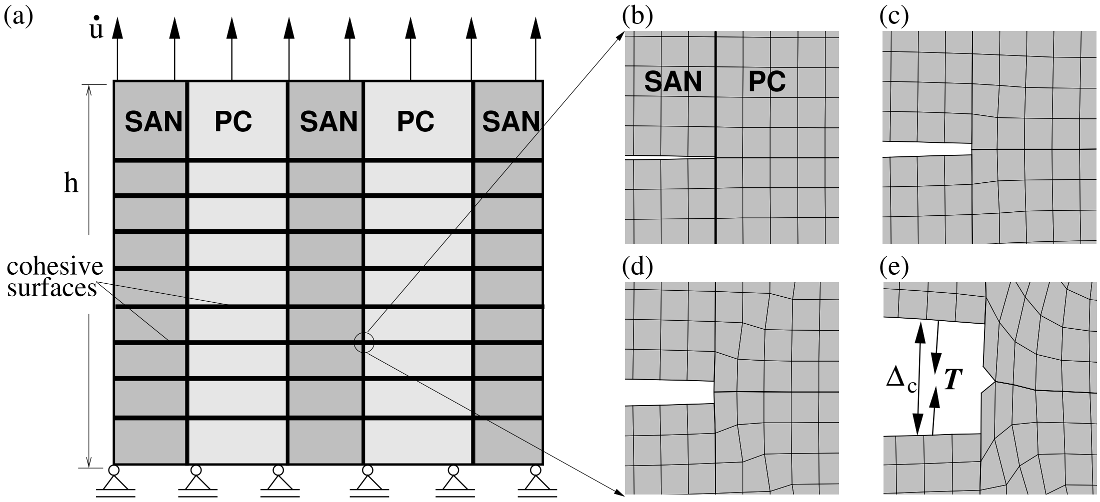

Figure 1: Modelling PC/SAN multilayer composites under tensile loading: (a) overall model set-up, (b)-(e) finite element modelling of successive craze/crack opening at PC/SAN interface

Constitutive models

In order to describe the large strain deformation behaviour of PC the constitutive model by Boyce et al. [3] is employed in the present work. The model accounts for intrinsic softening upon yield (which promotes the formation of shear bands) as well as progressive rehardenig due to stretching of the molecular (entanglement) network (see Fig. 2a). The deformation behaviour of SAN is taken linear elastic up to craze initiation.

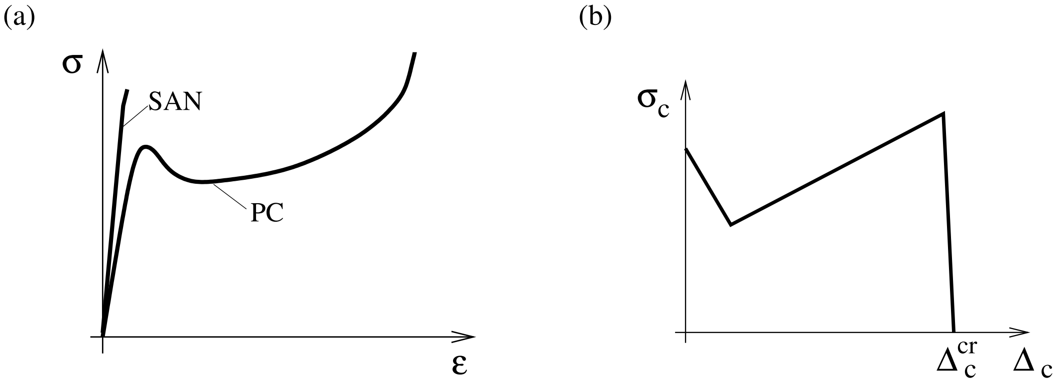

Figure 2: (a) Uniaxial response of the two bulk glassy polymers, (b) variation of craze widening resistance with craze opening displacement (thickness) in cohesive model for SAN

Crazing and the subsequent formation of cracks in the brittle SAN layers is described using a modified version of the cohesive surface model developed in [4]. Upon craze initiation (at a critical value of the local normal stress on the cohesive surface) the response of the fibrillated craze matter is represented on the continuum level by the separation $\boldsymbol{\Delta}_c$ of the craze-bulk interfaces (craze width) and the cohesive traction $\boldsymbol{T}$ as sketched in Fig. 1e. The relation between these two quantities is mainly governed by the craze widening resistance σ_c which – in contrast to the assumption of being constant made in [4] – is here taken to vary in the course of craze widening as sketched in Fig. 2b. The initial decrease of the craze widening resistance is attributed to the transformation of the material in the craze into thin “mature” fibrils while the later increase reflects an increasing resistance against drawing in of new material from the bulk. Full details of the bulk and cohesive constitutive models and values of the material parameters are given in [6].

Numerical Results

In the following we consider two different multilayer composites, one with a PC/SAN composition (i.e. relative layer thickness) of 3/1 ("PC-rich") and one with a composition of 1/3 ("SAN-rich"), both under uniaxial overall loading. A spatially random distribution of initial defects is modelled by some scatter (±10%) of the local craze initiation stress in the SAN. Numerical results in terms of contours of the local plastic strain are shown for the PC-rich composite at two successive levels of overall deformation in Figs. 3a and b and for the SAN-rich composite in Fig. 3c. Inelastic deformation starts by the formation of isolated crazes in the SAN layers. This induces local stress concentrations in the adjacent PC leading to the initiation of shear bands (dark diagonal zones in Fig. 3a). As the shear bands spread in the PC they impinge neighbouring PC/SAN interfaces and in turn induce stress concentrations in the SAN which cause the formation of new crazes. Figure 3b clearly shows an increased number of "defects" in the SAN which under continued overall deformation have evolved from crazes into cracks and even holes. The important point is that in PC-rich composites these local damage zones in the SAN (interconnected by shear bands in the PC) are uniformly distributed throughout the sample (Fig. 3a and b) whereas in SAN-rich composites (Fig. 3c) a localisation of damage and plastic deformation occurs.

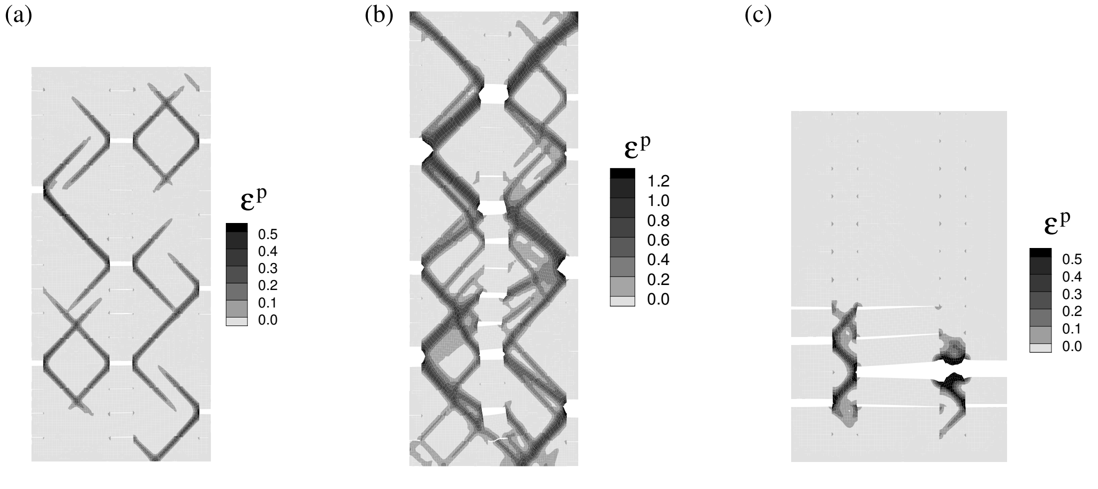

Figure 3: Patterns of local plastic deformation and damage in PC-rich composite (PC/SAN = 3/1) at (a) 7 % and (b) 20 % overall strain and in SAN-rich composite (PC/SAN = 1/3) at 7 % overall strain (c)

The overall response of the PC-rich and the SAN-rich composites is depicted in Fig. 4 in terms of the macroscopic stress $\bar{\sigma}$ (loading of the sample) versus macroscopic strain $\bar{\varepsilon}$. Here, results of several simulations with different, yet statistically equivalent, realisations of the initial defect distribution are included and show a good reproducability. Corresponding to the spatially uniform extension of a network of interacting crazes and shear bands visible in Figs. 3a and b, the PC-rich composites display a ductile overall behaviour. The SAN-rich composites, in contrast, undergo overall failure at small macroscopic strains due to the localisation of inelastic deformation visible in Fig. 3c.

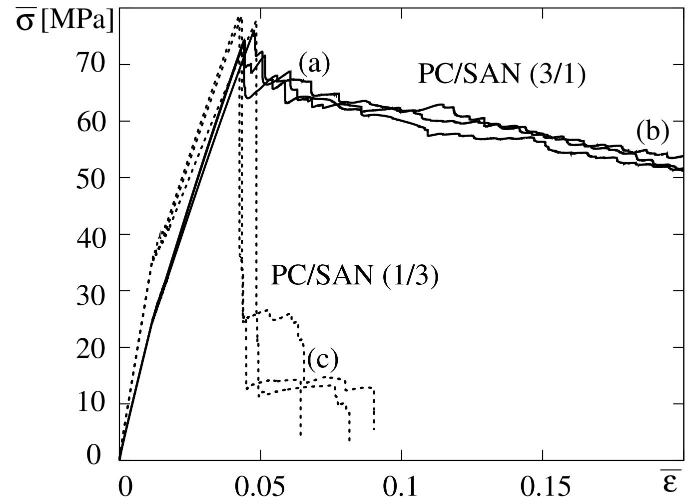

Figure 4: Overall response of PC-rich (3/1) and SAN-rich (1/3) composites under uniaxial tension; (a), (b), (c) correspond to contour plots in Fig. 3

Discussion

Multilayer composites of PC and SAN subjected to tensile loading have been investigated numerically utilising appropriate continuum mechanical constitutive models for the deformation and failure of both constituents. The simulation results well reproduce the experimentally observed local and overall response, i.e. the interaction of crazing/cracking in the SAN with shear banding in the PC on the microscale as well as the composition-dependent macroscopic brittle-to-ductile transition. Within the present 2D analyses, it turned out that an overall ductile behaviour of the composite is accompanied by the formation of a network of crazes/cracks interconnected by shear bands throughout large regions of the material. The key parameter for this to occur is the thickness of the PC layers relative to the SAN layers, since the shear bands in the PC “serve” to delocalize the damage in the neighbouring SAN by creating new stress concentrations and defects at some distance away from previous ones. It has, however, to be mentioned that from 3D analyses in [5] it was conjectured that tunnelling of surface crazes into the bulk also plays an important role.

Acknowledgements

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