Karlsruhe Institute of Technology

Institute of Mechanics

Multiscale Modeling of Deformation and Failure in ABS-Materials

Martin Helbig, Thomas Seelig

13. Problemseminar

„Deformation und Bruchverhalten von Kunststoffen"

Merseburg, Juni 2011

Institute of Mechanics
Kaiserstr. 12
D-76131 Karlsruhe
Tel.: +49 (0) 721/ 608-42071
Fax: +49 (0) 721/608-47990
E-Mail: info@ifm.kit.edu
www.ifm.uni-karlsruhe.de

Multiscale Modeling of Deformation and Failure in ABS-Materials

M. Helbig, Th. Seelig
Institute of Mechanics, Karlsruhe Institute of Technology, Karlsruhe

Summary: Deformation and failure mechanisms in ABS materials are investigated on various length scales utilizing continuum-micromechanical models and numerical (finite element) simulations.

Introduction

ABS (acrylonitrile-butadiene-styrene) is a prominent member of the class of so-called rubber-toughened thermoplastics, and it is widely used in technical products. Its most advantageous property, compared to neat thermoplastics, is the enhanced fracture toughness. The latter results from the heterogeneous composition and microstructure of ABS which consists of a glassy thermoplastic matrix (SAN, styrene-acrylonitrile) and fine dispersed sub-micron sized rubber (butadiene) particles (e.g. Bucknall, 1977). Generally speaking, the rubber particles serve to initiate inelastic (dissipative) micromechanisms at many sites throughout the material, such as void growth (upon rubber cavitation), shear yielding, and crazing. Despite numerous experimental studies, many details of these micromechanisms, their individual contribution to the overall toughness, and their dependence on microstructural parameters (e.g. size and volume fraction of the rubber particles) are still not very well understood. Theoretical models and numerical simulations are believed to provide a deeper insight into these issues. In the present work, several such modeling approaches – focusing on different length scales, yet all in the framework of continuum mechanics – are presented and discussed.

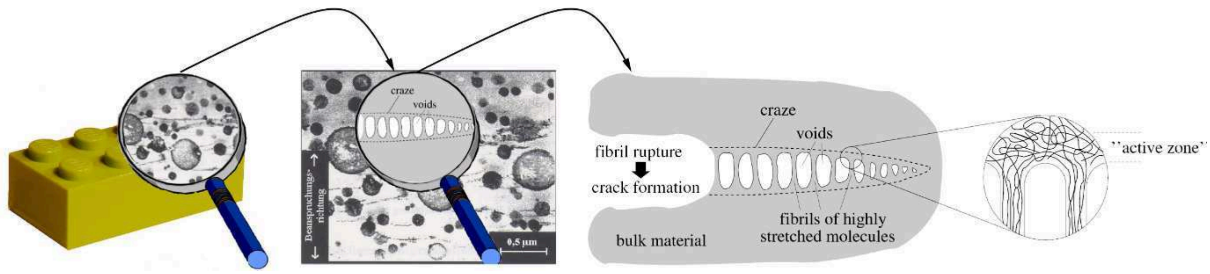

Figure 1: Microstructure and damage mechanisms in ABS; foto from (Grellmann & Seidler, 2001)

Constitutive model for amorphous thermoplastic polymers

The continuum-micromechanical models considered in the following sections require a proper description of the elastic-viscoplastic deformation behavior of the thermoplastic matrix material. The rheological model sketched in Fig. 2a illustrades such a description accounting for an elastic behavior at small strains, coupled with nonlinearly viscous flow counteracted by an internal (back) stress $\boldsymbol{b}$ due to progressive alignment of the molecular network at large strains (Haward & Thackray, 1968). The uniaxial response of the constitutive model, which here is used in the three-dimensional formulation by (Boyce et al., 1988), is sketched in Fig. 2b.

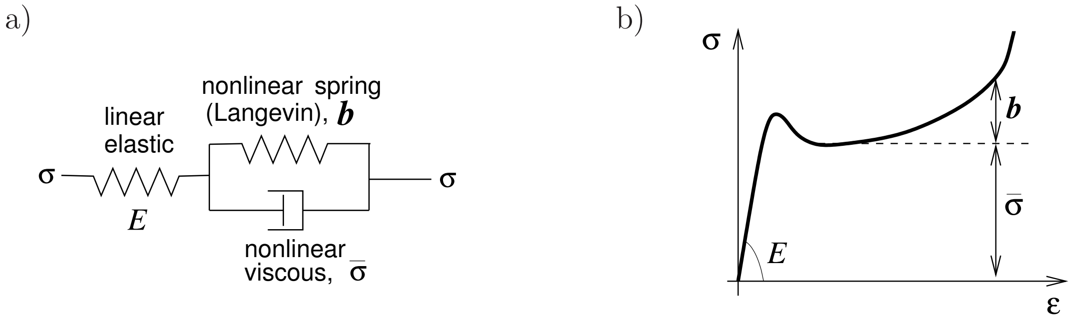

Figure 2: a) Rheological model for the elastic-viscoplastic deformation behavior of thermoplastic polymers, b) uniaxial stress-strain response

Micromechanical study of fibrillation

The damage mechanism on the perhaps finest length scale accessible to continuum mechanical modeling is the fibrillation of thermoplastic polymers under tensile loading. Fibrillation of a polymer material is found in various situations such as the failure of adhesive layers (Fig. 3a) or during crazing (Fig. 1). It is preceded by the growth and coalescence of microvoids (originating from microscale heterogeneities) and takes place by drawing of the polymer material between the voids. This drawing into fibrils is enabled by the progressive hardening (see Fig. 2b) that results from stretching of the molecular network. The mechanical effect of a network of polymer chains is essentially characterized by the number N of molecular units between entanglements points; the limit extensibility and hence maximum continuum stretch possible is then given by $\sqrt{N}$.

A numerical analysis of the fibrillation process in amorphous thermoplastic polymers has been performed in (Helbig & Seelig, 2011), based on micromechanical (cell) models which account for void coalescence, controlled by a local failure strain $\varepsilon^{\text{fail}}$, and the subsequent stretching of the matrix material into fibrils (Fig. 3b,c). The overall stress-strain response of such a cell model is shown in Fig. 4 for various values of the network parameter N.

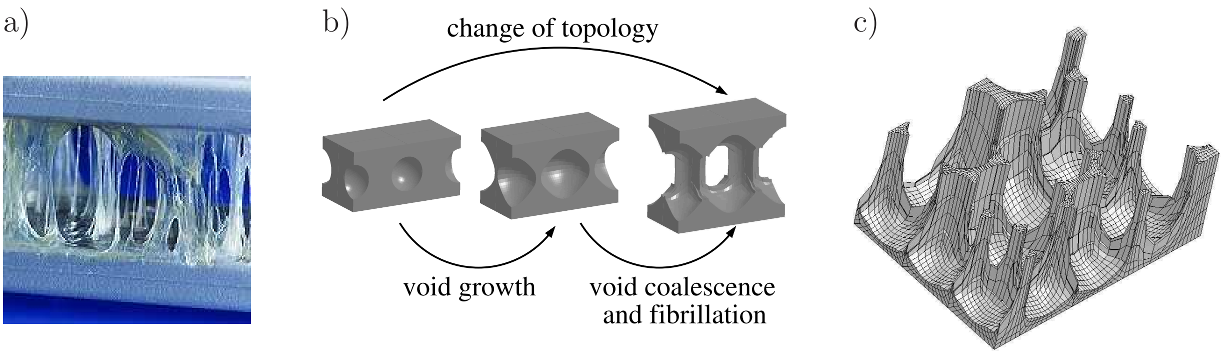

Figure 3: a) Fibrillation in adhesive layer (Fraunhofer IFAM), b) schematic of change of topology from isolated voids in continuous matrix to interconnected void space with isolated fibrils, c) deformed finite element model of a layer with initially irregular void arrangement

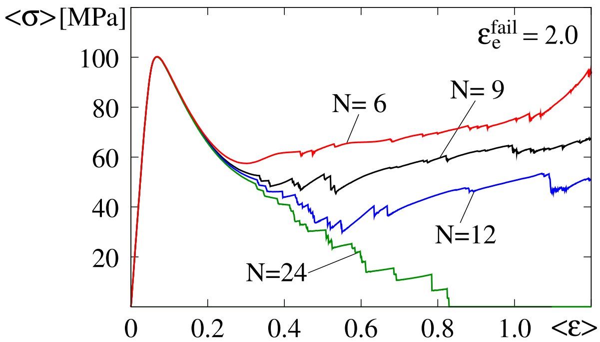

Figure 4: Overall response showing effect of network parameter N

Cohesive zone modeling of crazing

On a larger length scale, the formation and growth of crazes is of interest. Crazes are localized zones of fibrillated polymer material which transfer stress due to the load-carrying capacity of the numerous fibrils they consist of. They form normal to the direction of maximum principal tensile stress once a critical (tensile or hydrostatic) stress in the bulk thermoplastic polymer is reached. Under continued loading their growth and widening proceeds until at a critical craze thickness (fibril length), typically of the order of a micron, rupture of the fibrils takes place and a craze turns into a microcrack. Owing to their appearance as thin crack-like defects, crazes can be modeled as cohesive zones (Tijssens et al., 2000). Their mechanical behavior is then described by a traction-separation law which represents the "smeared" behavior of the fibrillated craze matter (Fig. 5). Different variations of the craze stress σ_c with the craze widening Δ_c are possible concerning the level of craze initiation stress as well as the craze hardening behavior (Fig. 5b).

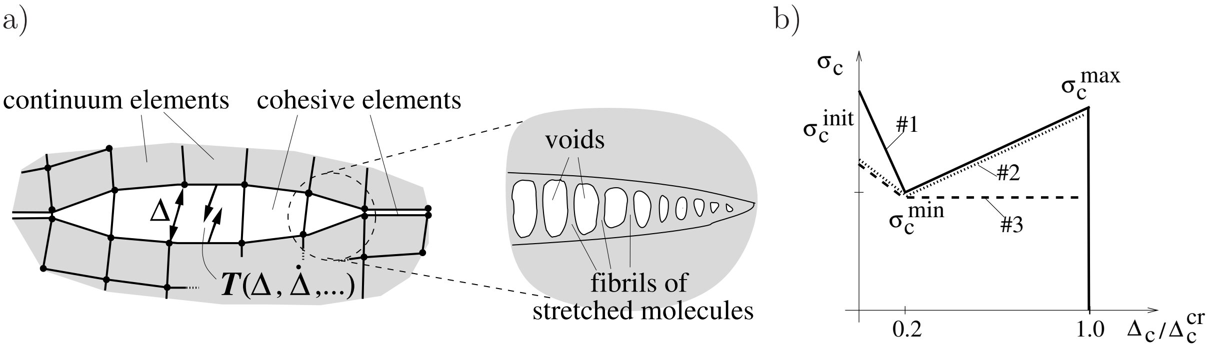

Figure 5: a) Cohesive zone modeling of crazing in a continuum mechanical setting, b) different cohesive (traction-separation) laws considered

Competition between void growth and crazing

Crazes preferentially initiate at stress concentrators such as rubber particles, and their interaction with (shear) yielding of the surrounding matrix is an interesting issue on the length scale of the particle-matrix microstructure of ABS. For instance, it is up to date not clear under which circumstances crazing *or* matrix yielding (enabled by void growth from cavitated rubber particles) are the dominant micromechanisms for the enhanced ductility and fracture toughness of ABS. Simulations therefore have been performed, considering a representative volume of the microstructure with several voids (cavitated rubber particles) interconnected by cohesive zones as potential locations for crazing.

Figure 6 shows results from 2D plane strain simulations for different crazing models in terms of the cohesive laws depicted in Fig. 5b. Findings from this study are as follows: When the craze initiation stress is high (#1), the dissipative micromechanisms occur

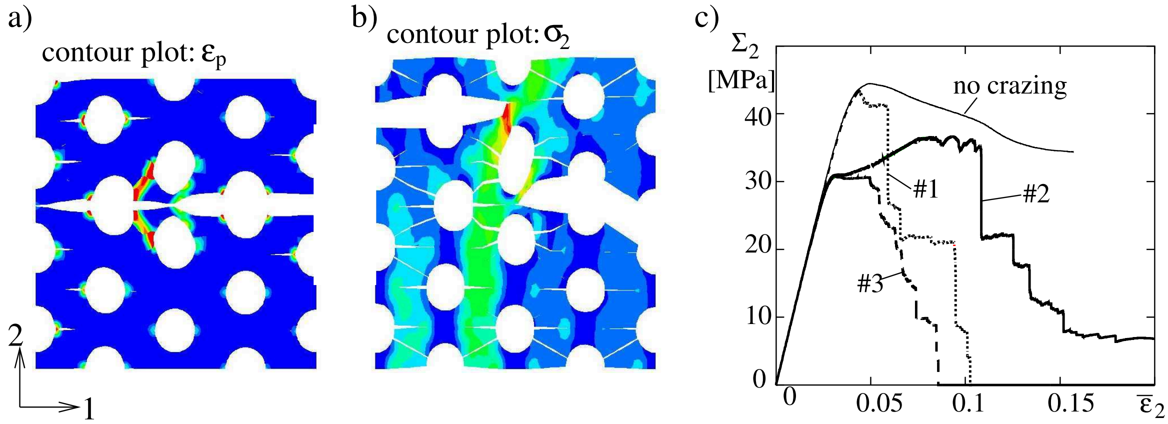

Figure 6: a) High craze initiation stress (#1 in Fig. 5b) leads to small amount of crazing and only localized matrix yielding, b) low craze initiation stress and craze hardening (#2 in Fig. 5b) leads to large amount of crazing, c) overall response in uniaxial straining

rather localized (see Fig. 6a) and lead to an early overall failure of the material (Fig. 6c). In contrast, a low craze initiation stress (#2) in conjunction with a craze hardening behavior at increasing Δ_c (as in model #1) results in a delocalized occurence of crazing (Fig. 6b) and a larger overall failure strain, i.e. an enhanced overall failure strain (Fig. 6c). Also shown in Fig. 6c is the response of the model in the extreme case when no crazing takes place and the imposed macroscopic strain is solely accommodated by void growth and matrix shear yielding. The softening overall response obtained in this case is contradictory to the behavior of real ABS.

A macroscopic model for distributed crazing

Motivated by the finding of the micromechanical study in the previous section that crazing plays a key role in the inelastic deformation behavior of ABS, a macroscopic constitutive model for the effect of distributed crazing has been set up. The contribution of crazing to the inelastic part of the strain rate tensor is given by

$$\boldsymbol{D}^c = \dot{\varepsilon}^c \, \boldsymbol{n} \otimes \boldsymbol{n} \qquad \text{with} \quad \dot{\varepsilon}^c = \dot{\varepsilon}_0 \exp\left(\frac{\phi}{A}\right) \qquad \text{and} \quad \phi = \boldsymbol{n} \cdot \boldsymbol{\sigma} \cdot \boldsymbol{n} - \sigma_c \tag{1}$$

where $\boldsymbol{n}$ is the unit vector in the direction of the maximum princial stress at the instant of craze initiation (i.e. normal to the evolving crazes), and $\dot{\varepsilon}_0$ and A are material constants. Distributed crazing hence is described in a homogenized manner as an anisotropic flow process ("craze yielding"). In analogy to the traction-separation relation of an individual craze (Fig. 5b), the overall yield strength in the homogenized model is taken to vary with the inelastic crazing strain: $\sigma_c = \sigma_c(\varepsilon^c)$.

Plastic zone at crack tip in rubber-toughended polymers

On the macroscopic scale of crack growth in a testing specimen or a technical component, the formation of the plastic zone at a crack tip is of interest with regard to the fracture resistance. Numerical simulations on that scale require a homogenized description of the material. With respect to ABS, different approaches have been investigated in a previous work (Pijnenburg et al., 2005), for instance a porous plasticity model that assumes void growth and matrix shear yielding as the dominant micromechanism. However, the key finding from that work was that the model overrated the effect of void growth and led to unrealistically narrow plastic zones.

Here, we alternatively focus on the effect of distributed crazing in the inelastic deformation of ABS and study the performance of the model described in the previous section. Figure 7a shows the computational model of a single edge notch tensile (SENT) specimen considered in the analysis of the plastic zone shape. Results are shown in Figs. 7b and c. In contrast to the homogeneous material description underlying Fig. 7b, a fine-scale spatial scatter of the craze yield strength is considered in Fig. 7c reflecting a nonuniform distribution of the microstructure (e.g. rubber particles in ABS). The total plastic zone obtained from this model contains numerous small finger-like localization zones (Fig. 7c) as are observed in experiments on amorphous (e.g. Ni et al., 1991; Ramaswamy & Lesser, 2002) as well as semi-crystalline (e.g. Kotter, 2003) rubber-roughened thermoplastics.

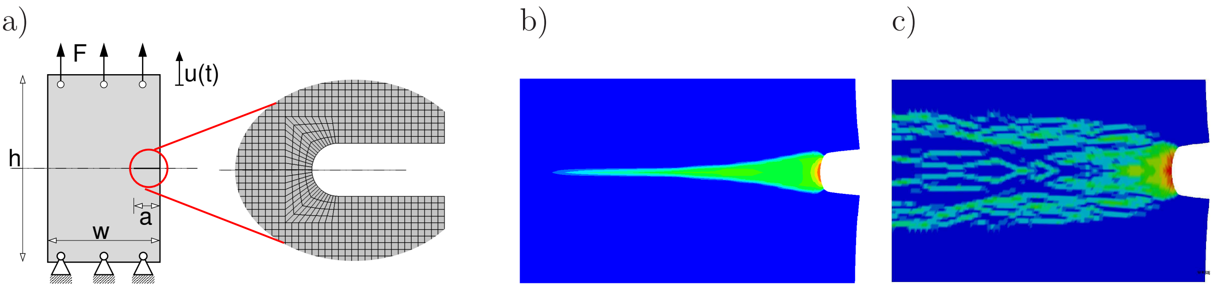

Figure 7: a) SENT specimen and finite element mesh at blunt crack tip; plastic zones at crack tip according to model for distributed crazing: a) material considered as homogeneous, b) with random variation of craze yield stress

Acknowledgment

Financial support of this work by the ,,Deutsche Forschungsgemeinschaft" (DFG) under grant no. SE 872/5 is gratefully acknowledged.

References

Boyce, M.C., Parks, D.M., Argon, A.S., 1988. Large inelastic deformation of glassy polymers. Part I: rate dependent constitutive model. Mech. Mater. 7, 15-33.

Bucknall, C.B., 1977. Toughened Plastics. Applied Science, London.

Grellmann, W., Seidler, S. (eds.), 2001. Deformation and fracture behaviour of polymers. Springer.

Haward, R.N., Thackray, G., 1968. The use of a mathematical model to describe isothermal stress-strain curves in glassy thermoplastics. Proc. Roy. Soc. A 302, 453-472.

Helbig, M., Seelig, Th., 2011. Micro-mechanical modeling of fibrillation in amorphous polymers. Computational Materials Science, in press.

Kotter, I., 2003. Morphologie-Zhigkeits-Korrelationen von EPR-modifizierten Polypropylenwerkstoffen. Dissertation, Halle-Wittenberg.

Ni, B.Y., Li, J.C.M. and Berry, V.K., 1991. Plastic zone in front of a mode I crack in acrylonitrile-butadiene-styrene polymers. Polymer 32, 2766-2770.

Pijnenburg, K.G.W., Seelig, Th., Van der Giessen, E., 2005. Successively refined models for crack tip plasticity in polymer blends. Eur. J. Mech. - A/Solids 24, 740-756.

Ramaswamy, S. and Lesser, A.J., 2002. Microscopic damage and macroscopic yield in acrylonitrile-butadiene styrene (ABS) resins tested under multi-axial stress states. Polymer 43, 3743-3752.

Tijssens, M.G.A., Van der Giessen, E. and Sluys, L.J., 2000. Modeling of crazing using a cohesive surface methodolgy. Mech. Mater. 32, 19-35.