MORPHOLOGY EVOLUTION MECHANISMS IN POLYURETHANE MATERIALS STUDIED BY SMALL-ANGLE X-RAY SCATTERING

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ABSTRACT

Polyurethanes (PU) are random block copolymer materials that can be adapted to an extremely wide range of applications. On the other hand, their manufacture requires the definition of parameters from a multidimensional space. Finally, the product shall have a morphology that meets the demand of the application. Instead of laborious production experiments it would be much easier to predict the properties of the material by a simulation program. In order to design the program we need to identify mechanisms in the response of the materials structure to typical loads (thermal, mechanical, environmental.). This can be done by monitoring the morphology evolution *in situ*. An appropriate tool is the small-angle X-ray scattering (SAXS).

Some results of a long-term project with industry cooperation are presented. In the project, the compositions of industrially relevant polyurethanes (PU) are systematically varied and the materials are processed under standard industrial conditions in a cooperation with BASF.

- Straining of all our materials above a strain of 50% is accomplished by a mechanism of “rupture-and relief”.
- A relation between polyol functionality, nanoscale morphology, and mechanical performance is presented.
- Above a strain of 60% the volume fraction of hard domains decreases linearly with increasing strain. The materials break as soon as the hard domains are disappeared.

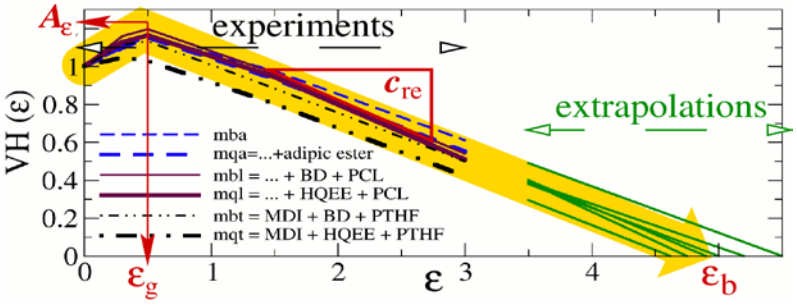

Figure 1. Variation of the relative volume fraction of hard domains, VH(ε) for $0 \leq \varepsilon \leq 3$ as determined from SAXS analysis. Characteristic parameters A_ε and ε_g are indicated. Linear extrapolations hit the ε-axis at the experimental strain-at-break ε_b.

- Melting and solidification at industrial rates is monitored by fast SAXS at a synchrotron source. The effect of nucleating agents on the nanostructure is reported. Clusters of nucleating agents are detected at high temperatures during the solidification branch.