Einladung zum Seminarvortrag im Aachener Mechanik & Statik Kolloquium

16. Oktober 2015; 10:00 Uhr;

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„Microstructure based Modelling of Elastomer Nano-Composites"

Prof. Dr. rer.nat.habil. Manfred Klüppel

Deutsches Institut für Kautschuktechnologie e.V.

In the first part of the talk the structure and dynamics of confined polymer between adjacent filler particles will be addressed, which plays a key role in understanding the mechanical properties of filler-reinforced elastomers. It will be demonstrated that several aspects of linear and non-linear viscoelasticity of filled rubbers can be traced back to the specific rate and temperature dependent properties of the confined polymer, forming glassy-like polymer bridges between adjacent filler particles. These filler-filler bonds consisting of immobilized polymer are quite stiff and transmit the stress under deformation of the filler network [1-5]. The pronounced non-linear behavior of filled elastomers is shown to be related to the rupture of glassy-like polymer bridges, which deform under strain and break if a critical strain is exceeded.

The rupture mechanism is described analytically in the frame of a microstructure-based model of rubber reinforcement, denoted Dynamic Flocculation Model, which will be described in some detail in the second part of the talk. In particular, the mechanical response due to cyclic breakdown and re-aggregation of tender filler clusters connected by glassy-like polymer bridges is formulated [6-9]. It allows for a microscopic understanding of the complex stress-strain properties during repeated, quasi-static deformations up to large strains, i.e. the well known filler induced stress softening and hysteresis effects. This is demonstrated by several examples of filler reinforced elastomers including systems filled with carbon nanotubes (CNT) and graphene nano-platelets (GNP).

Finally, the fracture mechanical properties of glassy-like polymer bridges under tension will be explored by a series of non-equilibrium molecular dynamics simulations of polymer films confined between two attractive solid walls [10-11]. These investigations provide a useful molecular tool for understanding the strongly non-linear mechanical response of filled elastomers. The estimated temperature behavior of the yield stress is found to be in fair agreement with experimental estimates of the tensile strength of filler-filler bonds (glassy-like polymer bridges), as obtained from adaptations of the quasi-static stress-strain response of carbon black filled SBR-rubber with the Dynamic Flocculation Model

Prof. Dr.-Ing. M. Itskov, Lehr- und Forschungsgebiet für Kontinuumsmechanik, RWTH Aachen
Prof. Dr.-Ing. habil. S. Klinkel, Lehrstuhl für Baustatik und Baudynamik, RWTH Aachen
Prof. Dr.-Ing. B. Markert, Institut für Allgemeine Mechanik, RWTH Aachen
Prof. Dr.-Ing. S. Reese, Institut für Angewandte Mechanik, RWTH Aachen
Prof. K. Veroy-Grepl Ph.D., AICES, RWTH Aachen