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MICROMECHANICAL MODELLING OF POLYMER NETWORKS TO SUPPORT THE DESIGN OF SELF-HEALING MATERIALS

Kapileswar Nayak[1] and Erik Van der Giessen[1]

[1]University of Groningen, Zernike Institute for Advance Materials (Micromechanics)
Dept. of Applied Physics, Nyenborgh 4, The Netherlands, 9747 AG.
Email: K.Nayak@rug.nl

ABSTRACT

This work is aimed at providing theoretical support and design tools for a novel approach to autonomous healing of polymer networks based on stress induced catalyst activation. A tetrahydrofurane (p-THF) network was prepared by crosslinking p-THF units through Silver-carbene complexes [1,2]. The idea is that when a sample is exposed to stress above a threshold level some crosslink breaks and catalyst is being activated. These active groups search for counter parts in the network to form a new crosslink.

To understand stress-induced catalyst activation we have developed a Finite Element Method (FEM) based quasi-static network model in a three-dimensional network contained in a representative volume element. For simplicity we take the network chains to be Freely Jointed Chains, with chain parameters that are obtained experimentally. The network structures are prepared by joining the p-THF units through different crosslink topologies. Both monodisperse and polydisperse (PDS) systems can be generated. These structures are then subjected to uniaxial tensile stretch and the stress-strain response is computed in dependence of the crosslink topology. Strain hardening is observed, which is due to (i) the finite extensibility of the chains and (ii) re-orientation of the chains in the strain direction. Comparison of monodisperse and PDS networks with identical crosslink topology shows that PDS networks are stiffer than the monodisperse ones.

During the simulation, we record the distribution of force in the chain for different networks at very small strain (0.02) and at a large strain (0.16). It is found that at small strains (2%) force-frequency histogram has a narrow distribution but the distribution gets wider at larger strain. We observed that a symmetric monodisperse network structure has a narrow distribution and force is relatively uniformly distributed throughout the network. On the other hand for the same crosslink topology, PDS networks have a broader distribution. From the stress-strain response and the force distribution observations we conclude that small chains attached to a crosslink of connectivity four is the weakest link inside the network. Hence crosslinks attached to those are expected to break first.

REFERENCES

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